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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].

Solving (8) by a well-known implicit scheme like BDF or Runge–Kutta methods requires in every step the solution of a nonlinear $n \times \ell$ matrix equation instead of the usual vector equation, and if one uses Newton's method, then the Jacobian of the vectorized matrix function with respect to the components of X must be (approximately) available. In general, unfortunately, the (numerical) approximation of this Jacobian is very complicated and costly; since in the computation of spectral intervals no explicit formula of F is available, the values of F at given points (t_i, X_i) are given only via a subroutine. If a good approximation to the Jacobian is not available, then a fixed-point iteration or a modified Newton iteration, see [14], must be used instead, which typically is slow and thus increases the computational cost significantly.

We will show that, by using half-explicit methods, these challenges can be mastered, since only the solution of a linear matrix equation in every time step is required.

The outline of the paper is as follows. In the following section, we propose half-explicit one-leg methods and analyze their convergence. Sections 3 and 4 contain the realization and the analysis of half-explicit variants of linear multistep methods and Runge–Kutta methods, respectively. It will be shown that, using the relation between the strangeness-free DAE (1) and the semi-explicit index-2 DAE (7), the half-explicit Runge–Kutta schemes proposed in this paper for (1) and those for (7) in [12] are equivalent. In Section 5, some numerical experiments illustrate the convergence results. We finish the paper with some conclusions.

2. Half-explicit one-leg (HEOL) methods for strangeness-free DAEs

In this section we discuss half-explicit one-leg (HEOL) methods which are special multistep methods. At time $t = t_N$, we use k previous approximations $x_{N-1}, \ldots, x_{N-k}$ for the computation of the approximation x_N to the solution value $x(t_N)$. Given real parameters α_j, β_j for $j = 0, 1, \ldots, k$, $\alpha_0 \neq 0$, a one-leg method for the numerical solution of an initial value problem associated with the ODE

$$\dot{x} = f(t, x) \tag{9}$$

is given by

$$\sum_{j=0}^{k} \alpha_j x_{N-j} = hf\left(\sum_{j=0}^{k} \beta_j t_{N-j}, \sum_{j=0}^{k} \beta_j x_{N-j}\right). \tag{10}$$

Here, if $\beta_0 = 0$, then we have an explicit method, otherwise an implicit method, and only one function evaluation of f per step is needed. Throughout this section, we suppose that $\beta_0 = 0$.

In order to have consistency for the scheme (10), we assume as in [16] that $\sum_{j=0}^{k} \alpha_j = 0$, $-\sum_{j=0}^{k} j\alpha_j = 1$, and $\sum_{j=1}^{k} \beta_j = 1$. Note that the last identity can always be achieved by a proper scaling of the coefficients β_i. The scheme (10) is *stable* if the associated characteristic polynomial $\rho(\lambda) = \sum_{j=0}^{k} \alpha_j \lambda^{k-j}$ is stable, i.e., all the roots of $\rho(\lambda)$ lie in the closed unit disk and the roots of modulus one are simple. Then the stability and consistency of order $p \geq 1$ implies the convergence of order p, see e.g. [5, Theorem 5.4].

The parameter set of a one-leg method can be adopted from that of linear multistep methods such as Euler methods, Adams methods, or BDF (backward differentiation formula) methods. The analysis of explicit one-leg methods applied to ODEs is presented, e.g., in [17,18]. For stiff ODEs and DAEs, however, one has to use implicit one-leg methods such as the implicit midpoint rule or BDF methods, see e.g. [1,4,5,19,16].

Here we adapt explicit one-leg methods in order to solve the strangeness-free DAE (1). For simplicity, in the analysis we assume that the mesh is uniform, i.e., that we have constant step-size. Using the concepts in [8, Section III.5], the analysis can be extended to the case of variable step-sizes as well.

If for (1) we apply an explicit one-leg discretization scheme to the differential part, which is scaled by h/α_0, and evaluate the algebraic equation at $t = t_N$, then in each time step we have to solve a nonlinear system $H_N(t_N, x_N, x_{N-1}, \ldots, x_{N-k}; h) = 0$ given by the equations

$$\begin{aligned} &(\mathrm{a})\ \frac{h}{\alpha_0} f\left(\sum_{j=1}^{k} \beta_j t_{N-j}, \sum_{j=1}^{k} \beta_j x_{N-j}, \frac{1}{h}\sum_{j=0}^{k} \alpha_j x_{N-j}\right) = 0, \\ &(\mathrm{b})\ g(t_N, x_N) = 0 \end{aligned} \tag{11}$$

for x_N. The Jacobian matrix of H_N with respect to x_N is

$$\frac{\partial}{\partial x_N} H_N(t_N, x_N, x_{N-1}, \ldots, x_{N-k}; h) = \begin{bmatrix} f_{\dot{x}}\left(\bar{t}_N, \sum_{j=1}^{k} \beta_j x_{N-j}, \frac{1}{h}\sum_{j=0}^{k} \alpha_j x_{N-j}\right) \\ g_x(t_N, x_N) \end{bmatrix}.$$

Note that $\bar{t}_N = \sum_{j=1}^{k} \beta_j t_{N-j}$ is usually different from t_N, but it remains close to t_N for sufficiently small h. Since the system is strangeness-free and f, g are assumed to be sufficiently smooth with bounded partial derivatives, the Jacobian matrix is boundedly invertible in the neighborhood of the exact solution for sufficiently small h. Then the system (11) has a locally unique solution x_N, which can be approximated by Newton's method, see e.g. [20]. The detailed analysis of the existence and uniqueness of the numerical solution by (11) is given in the proof of Theorem 1 below.

Note that, unlike the case of implicit methods ($\beta_0 \neq 0$), when we use the scheme (11), then the evaluation of $\partial f/\partial x$ at each step is avoided. Hence, if f and g are linear functions in $\dot{x}$ and x, respectively, as in (8), then (11) is a linear system for x_N.

For the semi-linear matrix-valued DAE (8), we then obtain

$$\frac{1}{\alpha_0}E_1(\bar{t}_N)\sum_{j=0}^{k}\alpha_j X_{N-j} = \frac{h}{\alpha_0}F\left(\bar{t}_N, \sum_{j=1}^{k}\beta_j X_{N-j}\right),$$
$$A_2(t_N)X_N = 0,$$

which we write as the linear system for X_N,

$$\begin{bmatrix} E_1(\bar{t}_N) \\ A_2(t_N) \end{bmatrix} X_N = \begin{bmatrix} -\frac{1}{\alpha_0}E_1(\bar{t}_N)\sum_{j=1}^{k}\alpha_j X_{N-j} + \frac{h}{\alpha_0}F\left(\bar{t}_N, \sum_{j=1}^{k}\beta_j X_{N-j}\right) \\ 0 \end{bmatrix}. \tag{12}$$

If one uses a direct solution method such as Gaussian elimination, then in each mesh-point $t = t_N$, only one LU factorization is needed to solve the linear matrix equation (12) instead of using Newton's method for a nonlinear system of essentially squared dimension.

In the following, we prove that the one-leg method (11) applied to (1) is convergent of order p provided that it is of order $p \geq 2$ and stable in the case of ODEs. For DAEs of the semi-linear form (8), we show convergence with $p = 1$, as well.

Theorem 1. *Suppose that the explicit one-leg method (10) as applied to ODEs (9) is convergent of order $p \geq 2$ (with starting values that are correct of order $\mathcal{O}(h^p)$). Then, the half-explicit scheme (11) applied to DAEs of the form (1) is convergent of order p as well, provided that the initial values are consistent. In the case of semi-linear DAEs (8), the scheme (12) is convergent with $p = 1$, as well.*

Proof. We use the same framework as in the proof for the convergence of BDF methods in [5, Theorem 5.27], but avoid the splitting of variables as we did in [21]. This in fact generalizes the state space form approach for the convergence analysis of numerical methods for semi-explicit DAEs of index 1, see [4, Chapter 6.1-2] and [5, p. 238]. Since the derivative of the algebraic variables is implicitly involved in the differential part, the convergence analysis for (1) is more complicated than in the semi-explicit case.

(a) *Existence and uniqueness of the numerical solution.* First, we prove the existence and the uniqueness of the numerical solution. We will prove that for all $N \geq k$ with $t_0 + Nh \leq t_f$, if $x_{N-j} = x^*(t_{N-j}) + \mathcal{O}(h^p)$ holds for $j = 1, \ldots, k$, then for sufficiently small h the nonlinear system (11) has a locally unique solution x_N that also satisfies $x_N = x^*(t_N) + \mathcal{O}(h^p)$.

The accuracy order of the one-leg method implies $\sum_{j=1}^{k}\beta_j x^*(t_{N-j}) = x^*(\bar{t}_N) + \mathcal{O}(h^p)$ and $\frac{1}{h}\sum_{j=0}^{k}\alpha_j x^*(t_{N-j}) = \dot{x}^*(\bar{t}_N) + \mathcal{O}(h^p)$, where $\bar{t}_N = \sum_{j=1}^{k}\beta_j t_{N-j}$. Consider the function H_N defined in (11) and consider a neighborhood of the exact solution defined by

$$\Gamma(h) = \left\{(\xi_N, \ldots, \xi_{N-k}), \xi_{N-j} \in \mathbb{R}^n, \|\xi_{N-j} - x^*(t_{N-j})\| \leq Ch^p, j = 0, 1, \ldots, k\right\}$$

with some positive constant C and $p \geq 2$. Then, for $(\xi_N, \ldots, \xi_{N-k}) \in \Gamma(h)$, we have

$$\begin{aligned}\frac{\partial}{\partial \xi_N}H_N(t_N, \xi_N, \ldots, \xi_{N-k}; h) &= \begin{bmatrix} f_{\dot{x}}\left(\bar{t}_N, \sum_{j=1}^{k}\beta_j\xi_{N-j}, \frac{1}{h}\sum_{j=0}^{k}\alpha_j\xi_{N-j}\right) \\ g_x(t_N, \xi_N) \end{bmatrix} \\ &= \begin{bmatrix} f_{\dot{x}}(\bar{t}_N, x^*(\bar{t}_N) + \mathcal{O}(h^p), \dot{x}^*(\bar{t}_N) + \mathcal{O}(h^{p-1})) \\ g_x(t_N, x^*(t_N) + \mathcal{O}(h^p)) \end{bmatrix} \\ &= \begin{bmatrix} f_{\dot{x}}(t_N, x^*(t_N), \dot{x}^*(t_N)) \\ g_x(t_N, x^*(t_N)) \end{bmatrix} + \mathcal{O}(h).\end{aligned}$$

Due to (2), there exists $h_0 > 0$ such that if $h \leq h_0$ then $\frac{\partial}{\partial \xi_N}H_N(t_N, \xi_N, \ldots, \xi_{N-k}; h)$ is nonsingular and its inverse is bounded by a constant independent of h. Due to the order assumption of the one-leg method, the exact solution $x^*(t)$ satisfies the equation

$$H_N(t_N, x^*(t_N), \ldots, x^*(t_{N-k}); h) = \mathcal{O}(h^{p+1}). \tag{13}$$

Thus, by the Implicit Function Theorem, the system (11) has a locally unique solution x_N. Furthermore, by linearizing $H_N(t_N, \xi_N, \ldots, \xi_{N-k}; h)$ about $(t_N, x^*(t_N), \ldots, x^*(t_{N-k}); h)$, it follows that there exists a constant $\mathcal{K}_0 > 0$ such that

$$\|x_N - x^*(t_N)\| \leq \mathcal{K}_0\left(\|x_{N-1} - x^*(t_{N-1})\| + \cdots + \|x_{N-k} - x^*(t_{N-k})\|\right) + \mathcal{O}(h^{p+1}) \tag{14}$$

holds. Thus, we immediately obtain that the numerical solution x_N also satisfies $x_N - x^*(t_N) = \mathcal{O}(h^p)$.

In this way, we have shown that (11) locally determines the numerical solution x_N, provided that the preceding numerical approximations $x_{N-j}, j = 1, \dots, k$, are sufficiently close to the exact solution. Let the unique solution x_N be defined by

$$x_N = \mathcal{S}(t_N, x_{N-1}, \dots, x_{N-k}; h), \tag{15}$$

then it follows from (11) that

$$H_N(t_N, \mathcal{S}(t_N, x_{N-1}, \dots, x_{N-k}; h), x_{N-1}, \dots, x_{N-k}; h) \equiv 0. \tag{16}$$

(b) *Consistency*. As second step, we show that (11), or equivalently (15), indeed gives a consistent numerical method. To this end, we define

$$\mathcal{X}_N = \begin{bmatrix} x_{N-1} \\ x_{N-2} \\ \vdots \\ x_{N-k} \end{bmatrix}, \qquad \mathcal{X}(t_N) = \begin{bmatrix} x^*(t_{N-1}) \\ x^*(t_{N-2}) \\ \vdots \\ x^*(t_{N-k}) \end{bmatrix},$$

together with

$$\mathcal{F}(t_N, \mathcal{X}_N; h) = \begin{bmatrix} \mathcal{S}(t_N, x_{N-1}, \dots, x_{N-k}; h) \\ x_{N-1} \\ \vdots \\ x_{N-k+1} \end{bmatrix}.$$

For consistency, we must study $\mathcal{X}(t_{N+1}) - \mathcal{F}(t_N, \mathcal{X}(t_N); h)$ and, therefore, consider

$$x^*(t_N) - \mathcal{S}(t_N, x^*(t_{N-1}), \dots, x^*(t_{N-k}); h).$$

By substituting $x_{N-j} = x^*(t_{N-j})$ for $j = 1, 2, \dots, k$, into the estimate (14) in Part (a), it immediately follows that this difference is of order $\mathcal{O}(h^{p+1})$, i.e.,

$$\left\| x^*(t_N) - \mathcal{S}(t_N, x^*(t_{N-1}), \dots, x^*(t_{N-k}); h) \right\| = \mathcal{O}(h^{p+1}). \tag{17}$$

This means that the discretization method (11) is consistent of order p.

(c) *Stability*. As the last step, we prove the stability of the method. For this, we must study $\mathcal{F}(t_N, \mathcal{X}(t_N); h) - \mathcal{F}(t_N, \mathcal{X}_N; h)$. Similar to the proof of [4, Theorem VII.3.5], we choose a sufficiently large constant C_0 and assume that the numerical solution satisfies the global estimates

$$\text{(i)} \ \left\| x_N - x^*(t_N) \right\| \le C_0 h \quad \text{and} \quad \text{(ii)} \ \left\| \frac{1}{h} \sum_{j=0}^{k} \alpha_j x_{N-j} - \dot{x}^*(\bar{t}_N) \right\| \le C_0 h \tag{18}$$

for all N with $t_0 + Nh \le t_f$ and all sufficiently small h. These estimates will be justified at the end of the proof. We again consider the first block

$$\mathcal{S}(t_N, x^*(t_{N-1}), \dots, x^*(t_{N-k}); h) - \mathcal{S}(t_N, x_{N-1}, \dots, x_{N-k}; h)$$

and determine the derivatives $\mathcal{S}_{x_{N-j}}$ of $\mathcal{S}$ with respect to x_{N-j} for $j = 1, 2, \dots, k$. Instead of (11), replacing the algebraic equation $g(t_N, x_N) = 0$ by $\sum_{j=0}^{N} \frac{\alpha_j}{\alpha_0} g(t_{N-j}, x_{N-j}) = 0$, we obtain

$$\begin{bmatrix} \dfrac{h}{\alpha_0} f\left(\bar{t}_N, \displaystyle\sum_{j=1}^{k} \beta_j x_{N-j}, \frac{1}{h}\left[\sum_{j=1}^{k} \alpha_j x_{N-j} + \alpha_0 \mathcal{S}(t_N, x_{N-1}, \dots, x_{N-k}; h) \right] \right) \\ \displaystyle\sum_{j=1}^{N} \frac{\alpha_j}{\alpha_0} g(t_{N-j}, x_{N-j}) + g(t_N, \mathcal{S}(t_N, x_{N-1}, \dots, x_{N-k}; h)) \end{bmatrix} = 0. \tag{19}$$

Differentiating (19) with respect to x_{N-j} for $j = 1, 2, \dots, k$, we get

$$\begin{bmatrix} \dfrac{\alpha_j}{\alpha_0} f_{\dot{x}} + f_{\dot{x}} \mathcal{S}_{x_{N-j}} + h \dfrac{\beta_j}{\alpha_0} f_x \\ \dfrac{\alpha_j}{\alpha_0} g_x + g_x \mathcal{S}_{x_{N-j}} \end{bmatrix} = 0,$$

where the Jacobian matrices $f_{\dot{x}}, f_x$ are evaluated at $(\bar{t}_N, \sum_{j=1}^{k} \beta_j x_{N-j}, \frac{1}{h} \sum_{j=0}^{k} \alpha_j x_{N-j})$ and the Jacobians g_x at (t_N, x_N) and (t_{N-j}, x_{N-j}), respectively. Due to the assumptions (2) and (18), for sufficiently small h, the matrix $\begin{bmatrix} f_{\dot{x}} \\ g_x \end{bmatrix}$ is boundedly invertible and $g_x(t_{N-j}, x_{N-j}) = g_x(t_N, x_N) + \mathcal{O}(h)$. Hence we have $\mathcal{S}_{x_{N-j}} = -\frac{\alpha_j}{\alpha_0} I_n + \mathcal{O}(h)$, and it follows that

$$\mathcal{S}(t_N, x^*(t_{N-1}), \ldots, x^*(t_{N-k}); h) - \mathcal{S}(t_N, x_{N-1}, \ldots, x_{N-k}; h) = \sum_{j=1}^{k} \left(-\frac{\alpha_j}{\alpha_0} I_n + \mathcal{O}(h) \right) (x^*(t_{N-j}) - x_{N-j}). \tag{20}$$

Thus,

$$\mathcal{F}(t_N, \mathcal{X}(t_N); h) - \mathcal{F}(t_N, \mathcal{X}_N; h) = \begin{bmatrix} \sum_{j=1}^{k} \left(-\frac{\alpha_j}{\alpha_0} I_n + \mathcal{O}(h) \right) (x^*(t_{N-j}) - x_{N-j}) \\ x^*(t_{N-1}) - x_{N-1} \\ \vdots \\ x^*(t_{N-k+1}) - x_{N-k+1} \end{bmatrix},$$

and we obtain the estimate

$$\|\mathcal{F}(t_N, \mathcal{X}(t_N); h) - \mathcal{F}(t_N, \mathcal{X}_N; h)\| \le (\|\mathcal{C}_\alpha \otimes I_n\| + \mathcal{K}_1 h) \|\mathcal{X}(t_N) - \mathcal{X}_N\|,$$

where

$$\mathcal{C}_\alpha = \begin{bmatrix} -\frac{\alpha_1}{\alpha_0} & \cdots & -\frac{\alpha_{k-1}}{\alpha_0} & -\frac{\alpha_k}{\alpha_0} \\ 1 & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 \end{bmatrix} \tag{21}$$

and the positive constant $\mathcal{K}_1$ is independent of h. If the underlying one-leg method is stable, then there exists a vector norm such that with the associated matrix norm, the inequality $\|\mathcal{C}_\alpha \otimes I_d\| \le 1$ is satisfied. Hence, the discretization method (11) is stable as well.

Combining the three parts of the proof, we conclude that the numerical solution x_N by (11) converges to the exact solution x^* with order p, i.e., there exists a positive constant C_1 such that

$$\left\| x_N - x^*(t_N) \right\| \le C_1 h^p$$

for all $N = 0, 1, \ldots,$ with $t_0 + Nh \le t_f$. In addition, combining the estimates (17) and (20) yields

$$\sum_{j=0}^{N} \alpha_j (x^*(t_{N-j}) - x_{N-j}) = \sum_{j=1}^{N} \mathcal{O}(h)(x^*(t_{N-j}) - x_{N-j}) + \mathcal{O}(h^{p+1}).$$

Let us recall that $\frac{1}{h} \sum_{j=0}^{N} \alpha_j x^*(t_{N-j}) = \dot{x}(\bar{t}_N) + \mathcal{O}(h^p)$. Thus, there exists a positive constant C_2 such that

$$\left\| \frac{1}{h} \sum_{j=0}^{N} \alpha_j x_{N-j} - \dot{x}^*(\bar{t}_N) \right\| \le C_2 h^p.$$

We note that the stability constant $\mathcal{K}_1$ and thus both C_1 and C_2 may depend on C_0. For $p \ge 2$, we can ensure the global estimates (18) by choosing h sufficiently small such that

$$C_1 h^{p-1} \le C_0 \quad \text{and} \quad C_2 h^{p-1} \le C_0.$$

Then, together with the assumption on the starting values, the global estimate (18) follows by induction. This finishes the proof of the convergence of the one-leg method (11) for the general strangeness-free nonlinear DAE (1).

Finally, we discuss the convergence of half-explicit one-leg methods as applied to strangeness-free semi-linear DAEs of the form (8). We need to solve a linear system (12) instead of a nonlinear system as in the general case. The coefficient of x_N (or X_N in the matrix-valued case) is $\begin{bmatrix} E_1(\bar{t}_N) \\ A_2(t) \end{bmatrix}$,which is nonsingular for all sufficiently small h due to (2). Thus, the existence of a *globally* unique numerical solution x_N for $h \le h_0$ with a sufficiently small $h_0 > 0$ holds without any preliminary assumption on the preceding approximates $x_{N-j}, j = 1, 2, \ldots, k$. Similarly, the system (19) inherits the semi-linear structure and therefore, the stability estimate (20) is obtained without the global assumption (18). This means that the restriction on p can be relaxed and the convergence of half-explicit one-leg methods holds for $p = 1$ as well. □

Remark 2. In the general case, because of the assumption (18), the above proof is valid only for $p \ge 2$. The only one-leg method with $k = p = 1$ is the half-explicit Euler method which is in fact the simplest method of the class of half-explicit Runge–Kutta methods discussed in Section 4. By exploiting the one-step property, the stability of this method holds without assuming (18). The convergence of half-explicit one-leg methods with $k \geq 2$ and $p = 1$ is still open, in general. However, for special cases such as for semi-linear strangeness-free DAEs of the form (8), which is just discussed here, and for semi-explicit DAEs of index 1, which is considered in [4], the convergence is established in the case $p = 1$ as well.

Remark 3. The stability condition for implicit one-leg methods applied to fully implicit DAEs of differentiation index 1, see [16, Theorem 1], is more restrictive, since the strict stability of the second characteristic polynomial is required in addition. See also the stability condition for half-explicit multistep methods given in the next section. Here, we have seen that, because of the special structure of (1) and the appropriate discretization of the algebraic part ((11)b), the half-explicit one-leg methods behave rather like BDF methods. Furthermore, instead of the discretization (11), one can use (provided that the starting values are consistent) the following equivalent discretization

$$\begin{bmatrix} \dfrac{h}{\alpha_0} f\left(\bar{t}_N, \displaystyle\sum_{j=1}^{k} \beta_j x_{N-j}, \frac{1}{h}\sum_{j=0}^{k} \alpha_j x_{N-j}\right) \\ \displaystyle\sum_{j=0}^{N} \frac{\alpha_j}{\alpha_0} g(t_{N-j}, x_{N-j}) \end{bmatrix} = 0.$$

Note that the second equation is exactly the direct discretization of the equation $\frac{d}{dt} g(t, x(t)) = 0$ by the one-leg method.

Example 4. The simplest example of a one-leg method is the explicit Euler method with $\alpha_0 = 1, \alpha_1 = -1$ and $\beta_1 = 1$, which is of order 1. If we apply the resulting half-explicit method to the test DAE [22]

$$\begin{bmatrix} 1 & -\omega t \\ 0 & 0 \end{bmatrix} \dot{x} = \begin{bmatrix} \lambda & \omega(1-\lambda t) \\ -1 & 1+\omega t \end{bmatrix} x, \tag{22}$$

then with stepsize h we obtain the generalized stability function

$$R(z, w) = \frac{1+z+w}{1+w},$$

where $z = \lambda h$ and $w = \omega h$. Comparing this with the stability function of the implicit Euler method, see [22],

$$R(z, w) = \frac{1-w}{1-z-w},$$

we may conclude that the half-explicit method is feasible for non-stiff DAEs of the form (1), i.e., DAEs where the underlying ODE is non-stiff. For the test equation (22), this means that λ has negative, but not too large real part.

Example 5. A family of second order two-step methods introduced in [17] is defined by the coefficients

$$\alpha_0 = \frac{1}{\xi}, \qquad \alpha_1 = 1 - \frac{2}{\xi}, \qquad \alpha_2 = \frac{1}{\xi} - 1, \qquad \beta_1 = \frac{1}{2} + \frac{1}{\xi}, \qquad \beta_2 = \frac{1}{2} - \frac{1}{\xi},$$

where ξ is a parameter, $0 < \xi \leq 2$. If $\xi = 1$, then we have the one-leg variant of the well-known two-step Adams–Bashforth scheme.

3. Half-explicit linear multistep methods

In this section we consider explicit linear multistep methods applied to (9) as basis for the construction of half-explicit linear multistep (HELM) methods. These take the form

$$\sum_{j=0}^{k} \alpha_j x_{N-j} = h \sum_{j=1}^{k} \beta_j f_{N-j}, \quad f_{N-j} = f(t_{N-j}, x_{N-j}). \tag{23}$$

Without loss of generality, we assume that $\alpha_0 = 1$ and $\beta_1 \neq 0$ (if β_1 is not zero, then we use the first non-zero parameter among the β_j instead). To construct a half-explicit method for (1), the only question is how to implement this method for the differential part. Using the idea introduced for implicit multistep methods for DAEs in [19], we proceed as follows. Let x_N and w_N be approximations of the exact solution $x(t_N)$ and its derivative $w(t_N) := \dot{x}(t_N)$, respectively. Now, suppose that we have already determined $x_{N-k}, \ldots, x_{N-1}$ and $w_{N-k}, \ldots, w_{N-2}$. The scheme (23) is equivalent to $\sum_{j=0}^{k} \alpha_j x_{N-j} = h \sum_{j=1}^{k} \beta_j w_{N-j}$, from which we get

$$w_{N-1} = \frac{1}{\beta_1}\left(\frac{1}{h}\sum_{j=0}^{k} \alpha_j x_{N-j} - \sum_{j=2}^{k} \beta_j w_{N-j}\right). \tag{24}$$

Using this approximate formula for w_{N-1}, we approximate the differential part at $t = t_{N-1}$ and the algebraic part at $t = t_N$. This results in a nonlinear system for x_N given by

$$f(t_{N-1}, x_{N-1}, w_{N-1}) = 0,$$
$$g(t_N, x_N) = 0,$$

or equivalently

$$\begin{aligned} &\text{(a) } h\beta_1 f\left(t_{N-1}, x_{N-1}, \frac{1}{\beta_1}\left(\frac{1}{h}\sum_{j=0}^{k}\alpha_j x_{N-j} - \sum_{j=2}^{k}\beta_j w_{N-j}\right)\right) = 0, \\ &\text{(b) } g(t_N, x_N) = 0. \end{aligned} \tag{25}$$

This system has a locally unique solution x_N for sufficiently small h which can be approximated by Newton's method. Applying (25) to the semi-linear DAE (8), we obtain the linear system

$$\begin{bmatrix} E_1(t_{N-1}) \\ A_2(t_N) \end{bmatrix} X_N = \begin{bmatrix} -E_1(t_{N-1})\left(\sum_{j=1}^{k}\alpha_j X_{N-j} - h\sum_{j=2}^{k}\beta_j W_{N-j}\right) + h\beta_1 F(t_{N-1}, X_{N-1}) \\ 0 \end{bmatrix}. \tag{26}$$

So, similar as for the half-explicit one-leg methods, we need to perform only one *LU* factorization per step to solve the system (26) for X_N. The derivative approximation W_{N-1} that is needed for the next step is obtained by (24).

Let us introduce the *second characteristic polynomial* $\sigma(\lambda) = \sum_{j=1}^{k}\beta_j\lambda^{k-j}$, which is associated with the formula (24). We will see below that, to ensure the stability of the numerical scheme, this polynomial has to be strictly stable, i.e., all the roots must be inside the open unit disk, in addition to the stability of ρ. Furthermore, to initialize the scheme (25), we need not only the starting values $x_j, j = 0, \ldots, k-1$, but also the starting values $w_j, j = 0, \ldots, k-2$.

We have the following convergence result for half-explicit linear multistep methods.

Theorem 6. *Suppose that the explicit linear multistep method (23) applied to an ODE of the form (9) is convergent of order $p \geq 2$ and that the second characteristic polynomial $\sigma(\lambda)$ is strictly stable. In addition, we assume that all the starting values are accurate of order p and consistent, i.e., they satisfy $g(t_j, x_j) = 0$ for $j = 0, \ldots, k-1$ and $f(t_j, x_j, w_j) = 0$ for $j = 0, \ldots, k-2$. Then, the half-explicit scheme (25) applied to the DAE (1) is convergent of order p as well. For semi-linear strangeness-free DAEs of the form (8), the convergence holds for $p = 1$ as well.*

Proof. We proceed in the same way as in the convergence analysis for half-explicit one-leg methods. Consider the nonlinear system (25). All the arguments for proving the existence of a locally unique numerical solution x_N and the consistency are similar but with some slight differences due to the appearance of the derivative approximations $w_{N-j}, j = 2, \ldots, k$. Let us introduce $x_N = \mathcal{S}(t_N, x_{N-1}, \ldots, x_{N-k}, w_{N-2}, \ldots, w_{N-k}; h)$ and $w_{N-1} = \mathcal{Q}(t_N, x_{N-1}, \ldots, x_{N-k}, w_{N-2}, \ldots, w_{N-k}; h)$ with solution operators $\mathcal{S}$ and $\mathcal{Q}$, respectively. The consistency analysis shows that, if $x_{N-j} = x^*(t_{N-j})$ for $j = 1, 2, \ldots, k$, and $w_{N-j} = \dot{x}^*(t_{N-j})$ for $j = 2, \ldots, k$, then

$$x^*(t_N) - \mathcal{S}(t_N, x_{N-1}, \ldots, x_{N-k}, w_{N-2}, \ldots, w_{N-k}; h) = \mathcal{O}(h^{p+1}) \tag{27}$$

and

$$\dot{x}^*(t_{N-1}) - \mathcal{Q}(t_N, x_{N-1}, \ldots, x_{N-k}, w_{N-2}, \ldots, w_{N-k}; h) = \mathcal{O}(h^p). \tag{28}$$

We also define

$$\mathcal{Z}_N = \begin{bmatrix} x_{N-1} \\ x_{N-2} \\ \vdots \\ x_{N-k} \\ w_{N-2} \\ \vdots \\ w_{N-k} \end{bmatrix}, \qquad \mathcal{Z}(t_N) = \begin{bmatrix} x^*(t_{N-1}) \\ x^*(t_{N-2}) \\ \vdots \\ x^*(t_{N-k}) \\ w^*(t_{N-2}) \\ \vdots \\ w^*(t_{N-k}) \end{bmatrix},$$

where w^* denotes the derivative of x^*, and

$$\mathcal{G}(t_N, \mathcal{Z}_N; h) = \begin{bmatrix} \mathcal{S}(t_N, x_{N-1}, \dots, x_{N-k}; h) \\ x_{N-1} \\ \vdots \\ x_{N-k+1} \\ \mathcal{Q}(t_N, x_{N-1}, \dots, x_{N-k}, w_{N-2}, \dots, w_{N-k}; h) \\ w_{N-2} \\ \vdots \\ w_{N-k+1} \end{bmatrix}.$$

We focus on proving the stability of the scheme (24), (25). Let us assume the global estimates

$$\text{(i)}\ \left\|x_N - x^*(t_N)\right\| \le C_3 h \quad \text{and} \quad \text{(ii)}\ \left\|w_N - \dot{x}^*(t_N)\right\| \le C_3 h \tag{29}$$

for all $N = 0, 1, \dots,$ with $t_0 + Nh \le t_f$, with some constant C_3, and for all sufficiently small h. Instead of (25), we consider the equivalent nonlinear system

$$\begin{aligned} &\text{(a)}\ h\beta_1 f\left(t_{N-1}, x_{N-1}, \frac{1}{\beta_1}\left(\frac{1}{h}\sum_{j=0}^{k}\alpha_j x_{N-j} - \sum_{j=2}^{k}\beta_j w_{N-j}\right)\right) = 0, \\ &\text{(b)}\ \sum_{j=0}^{k}\alpha_j g(t_{N-j}, x_{N-j}) = 0. \end{aligned} \tag{30}$$

Recall that here $\alpha_0 = 1$ is already assumed. Then, by differentiating (30), elementary calculations show that, under the global assumption (29), the Jacobians of $\mathcal{S}$ satisfy

$$\begin{bmatrix} f_{\dot{x}}\mathcal{S}_{x_{N-j}} + \alpha_j f_{\dot{x}} \\ g_x \mathcal{S}_{x_{N-j}} + \alpha_j g_x \end{bmatrix} = \mathcal{O}(h), \quad \text{hence } \mathcal{S}_{x_{N-j}} = -\alpha_j I_n + \mathcal{O}(h),\ 1 \le j \le k,$$

and

$$\begin{bmatrix} f_{\dot{x}}\mathcal{S}_{w_{N-j}} - h\beta_j f_{\dot{x}} \\ g_x \mathcal{S}_{w_{N-j}} \end{bmatrix} = 0, \quad \text{hence } \mathcal{S}_{w_{N-j}} = \begin{bmatrix} f_{\dot{x}} \\ g_x \end{bmatrix}^{-1} \begin{bmatrix} h\beta_j f_{\dot{x}} \\ 0 \end{bmatrix} = \mathcal{O}(h),\ 2 \le j \le k. \tag{31}$$

Consequently, we obtain the estimate

$$\begin{aligned} &\mathcal{S}(t_N, x^*(t_{N-1}), \dots, w^*(t_{N-k}); h) - \mathcal{S}(t_N, x_{N-1}, \dots, w_{N-k}; h) \\ &\quad = \sum_{j=1}^{k}(-\alpha_j I_n + \mathcal{O}(h))(x^*(t_{N-j}) - x_{N-j}) + \sum_{j=2}^{k}\mathcal{O}(h)(w^*(t_{N-j}) - w_{N-j}). \end{aligned} \tag{32}$$

The estimates for $\mathcal{Q}_{x_{N-j}}$ and $\mathcal{Q}_{w_{N-j}}$ are obtained as follows. Substituting $x_N = \mathcal{S}(t_N, x_{N-1}, \dots, w_{N-k}; h)$ into (24) and differentiating with respect to x_{N-j} and w_{N-j}, we have

$$\mathcal{Q}_{x_{N-j}} = \frac{1}{\beta_1 h}(\mathcal{S}_{x_{N-j}} + \alpha_j I_n) = \frac{1}{\beta_1 h}(-\alpha_j I_n + \mathcal{O}(h) + \alpha_j I_n) = \mathcal{O}(1)$$

for $1 \le j \le k$ and

$$\mathcal{Q}_{w_{N-j}} = \frac{1}{\beta_1 h}\mathcal{S}_{w_{N-j}} - \frac{\beta_j}{\beta_1} I_n$$

for $2 \le j \le k$. Then (31) implies that

$$\frac{1}{\beta_1 h}\mathcal{S}_{w_{N-j}} = \begin{bmatrix} f_{\dot{x}} \\ g_x \end{bmatrix}^{-1} \begin{bmatrix} \frac{\beta_j}{\beta_1} f_{\dot{x}} \\ 0 \end{bmatrix}.$$

On the other hand, by linearizing $f(t_{N-j}, x_{N-j}, w_{N-j}) = 0$ at $(t_{N-j}, x^*(t_{N-j}), w^*(t_{N-j}))$ for $j \ge 2$, and again making use of (29), we obtain

$$(f_{\dot{x}} + \mathcal{O}(h))(w^*(t_{N-j}) - w_{N-j}) = -(f_x + \mathcal{O}(h))(x^*(t_{N-j}) - x_{N-j}).$$

This leads to the estimate

$$\mathcal{Q}(t_N, x^*(t_{N-1}), \dots, w^*(t_{N-k}); h) - \mathcal{Q}(t_N, x_{N-1}, \dots, w_{N-k}; h)$$
$$= \sum_{j=1}^{k} \mathcal{O}(1)(x^*(t_{N-j}) - x_{N-j}) + \sum_{j=2}^{k} \left(-\frac{\beta_j}{\beta_1} + \mathcal{O}(h) \right) (w^*(t_{N-j}) - w_{N-j}). \tag{33}$$

Summarizing the estimates (32) and (33), it then follows that

$$\mathcal{G}(t_N, \mathcal{Z}(t_N); h) - \mathcal{G}(t_N, \mathcal{Z}_N; h)$$
$$= \begin{bmatrix} \sum_{j=1}^{k} \left(-\frac{\alpha_j}{\alpha_0} I_n + \mathcal{O}(h) \right) (x^*(t_{N-j}) - x_{N-j}) + \sum_{j=2}^{k} \mathcal{O}(h)(w^*(t_{N-j}) - w_{N-j}) \\ x^*(t_{N-1}) - x_{N-1} \\ \vdots \\ x^*(t_{N-k+1}) - x_{N-k+1} \\ \sum_{j=1}^{k} \mathcal{O}(1)(x^*(t_{N-j}) - x_{N-j}) + \sum_{j=2}^{k} \left(-\frac{\beta_j}{\beta_1} I_N + \mathcal{O}(h) \right) (w^*(t_{N-j}) - w_{N-j}) \\ w^*(t_{N-2}) - w_{N-2} \\ \vdots \\ w^*(t_{N-k+1}) - w_{N-k+1} \end{bmatrix},$$

and equivalently, we have

$$\mathcal{G}(t_N, \mathcal{Z}(t_N); h) - \mathcal{G}(t_N, \mathcal{Z}_N; h) = \begin{bmatrix} \mathcal{C}_\alpha \otimes I_n + \mathcal{O}(h) & \mathcal{O}(h) \\ \mathcal{O}(1) & \mathcal{C}_\beta \otimes I_n + \mathcal{O}(h) \end{bmatrix} (\mathcal{Z}(t_N) - \mathcal{Z}_N),$$

where $\mathcal{C}_\alpha$ is defined by (21) and

$$\mathcal{C}_\beta = \begin{bmatrix} -\frac{\beta_2}{\beta_1} & \cdots & -\frac{\beta_{k-1}}{\beta_1} & -\frac{\beta_k}{\beta_1} \\ 1 & \ddots & 0 & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 \end{bmatrix}.$$

Because of the stability of $\rho(\lambda)$ and the strict stability of $\sigma(\lambda)$, there exists a norm such that $\|\mathcal{C}_\alpha \otimes I_d\| = 1$ and $\left\|\mathcal{C}_\beta \otimes I_n\right\| = \kappa < 1$. Let us partition $\mathcal{G} = (\mathcal{G}^{(1)^T}, \mathcal{G}^{(2)^T})^T$ according to the size of $\mathcal{C}_\alpha \otimes I_n$ and $\mathcal{C}_\beta \otimes I_n$. Similarly, we partition $\mathcal{Z} = (\mathcal{Z}^{(1)^T}, \mathcal{Z}^{(2)^T})^T$ and $\mathcal{Z}_N = (\mathcal{Z}_N^{(1)^T}, \mathcal{Z}_N^{(2)^T})^T$ and obtain

$$\begin{bmatrix} \left\|\mathcal{G}^{(1)}(t_N, \mathcal{Z}(t_N); h) - \mathcal{G}^{(1)}(t_N, \mathcal{Z}_N; h)\right\| \\ \left\|\mathcal{G}^{(2)}(t_N, \mathcal{Z}(t_N); h) - \mathcal{G}^{(2)}(t_N, \mathcal{Z}_N; h)\right\| \end{bmatrix} \le \begin{bmatrix} 1 + \mathcal{O}(h) & \mathcal{O}(h) \\ \mathcal{O}(1) & \kappa + \mathcal{O}(h) \end{bmatrix} \begin{bmatrix} \left\|\mathcal{Z}^{(1)}(t_N) - \mathcal{Z}_N^{(1)}\right\| \\ \left\|\mathcal{Z}^{(2)}(t_N) - \mathcal{Z}_N^{(2)}\right\| \end{bmatrix}.$$

Using the same technique as that in the proof of [4, Lemma VI.3.9], we obtain that there exist a norm and a positive constant $\mathcal{K}_2$ such that

$$\|\mathcal{G}(t_N, \mathcal{Z}(t_N); h) - \mathcal{G}(t_N, \mathcal{Z}_N; h)\| \le (1 + \mathcal{K}_2 h) \|\mathcal{Z}(t_N) - \mathcal{Z}_N\|.$$

Hence, the discretization method (24)–(25) is stable. Combining with the local error estimates (27) and (28), [4, Lemma VI.3.9] shows that both x_N and w_{N-1} converge to the exact values $x^*(t_N)$ and $\dot{x}^*(t_{N-1})$, respectively, with the same order p. In other words, there exist positive constants C_4 and C_5 such that

$$\left\|x^*(t_N) - x_N\right\| \le C_4 h^p \quad \text{and} \quad \left\|\dot{x}^*(t_{N-1}) - w_{N-1}\right\| \le C_5 h^p.$$

Since $p \ge 2$ is assumed, with sufficiently small h, the validity of the global estimates (29) follows by induction.

Finally, for semi-linear DAEs (8), the resulting system (26) that is to be solved is linear. Thus, by similar arguments as in the proof of Theorem 1, the convergence of the discretization scheme (26) is extended to the case $p = 1$, too. □

Remark 7. We stress that, similar to the case of one-leg methods, the restriction $p \ge 2$ can be relaxed if the half-explicit multistep methods (25) is applied to semi-explicit DAEs of index 1 or to semi-linear strangeness-free DAEs like (8). The implementations of HELM methods in these special cases are simpler. For example, in the case of semi-explicit DAEs of index 1, one first calculates the differential component explicitly, then solves the algebraic equation for the algebraic component.

This means that the introduction of the auxiliary variables w_N and its recursion (24) can be avoided. Furthermore, by the state space form approach, the convergence of the numerical solution is easily verified which does not require the extra condition on the second characteristic polynomial, see [4, pp. 376,383].

Example 8. A family of second order two-step methods, introduced in [17], is defined by

$$\alpha_0 = 1, \qquad \alpha_1 = \xi - 2, \qquad \alpha_2 = 1 - \xi, \qquad \beta_1 = \frac{\xi}{2} + 1, \qquad \beta_2 = \frac{\xi}{2} - 1,$$

where ξ is a parameter, $0 < \xi \le 2$. It is easy to verify that for each $\xi \in (0, 2]$, the half-explicit methods (25) based on these schemes satisfy the conditions of Theorem 6 with convergence order $p = 2$. If $\xi = 1$, then we obtain the well-known 2-step Adams–Bashforth formula.

Example 9. Consider the 3-step Adams–Bashforth method

$$\alpha_0 = 1, \qquad \alpha_1 = -1, \qquad \alpha_2 = \alpha_2 = 0, \qquad \beta_1 = 23/12, \qquad \beta_2 = -4/3, \qquad \beta_3 = 5/12,$$

which is well known to be convergent of order $p = 3$ as applied to ODEs [8]. It is easy to check that $\sigma(\lambda)$ is strictly stable, thus the half-explicit method (25) based on this scheme is convergent of order $p = 3$ as applied to (1). Similarly, by Theorem 6, one can verify without difficulty that the half-explicit 4- and 5-step Adams–Bashforth methods are convergent of order $p = 4, 5$, respectively. In contrast, Adams–Moulton schemes, the well-known implicit counterparts, are unstable when applied to DAEs, since their second characteristic polynomial is not stable, see [4,23]. Thus, surprisingly, explicit Adams–Bashforth schemes, implemented appropriately in the half-explicit framework (25), are feasible for solving (non-stiff) DAEs (1). It is also straightforward to extend the half-explicit linear multistep methods proposed here to semi-explicit index-2 DAEs (7), i.e., they are alternative candidates for solving this class of DAEs, in addition to BDF and difference corrected multistep methods [24,4].

4. Half-explicit Runge–Kutta methods

For a given explicit Runge–Kutta method, the corresponding half-explicit Runge–Kutta (HERK) method can be constructed using a similar idea as in the case of half-explicit linear multistep methods. However, for the convergence analysis, we will exploit the equivalence between (1) and (7) and make use of the well-known order conditions and convergence results of half-explicit Runge–Kutta methods that exist for semi-explicit index-2 DAEs, [12,3]. Consider an s-stage explicit Runge–Kutta method given by Table 1 with $c_1 = 0$. We assume that $a_{i+1,i} \neq 0$ for $i = 1, \dots, s-1$ and $b_s \neq 0$. Consider an interval $[t_{N-1}, t_N]$ and suppose that an approximation x_{N-1} to $x(t_{N-1})$ is given. Let $\Xi_i \approx x(t_{N-1} + c_i h)$ be the stage approximation and let $K_i = \dot{\Xi}_i$ be the approximations to the derivatives of Ξ_i, $i = 1, \dots, s$. Then, the explicit Runge–Kutta scheme defined by Table 1 reads

$$\begin{aligned}
&\text{(a) } \Xi_1 = x_{N-1}, \\
&\text{(b) } \Xi_i = x_{N-1} + h\sum_{j=1}^{i-1} a_{i,j}K_j, \quad i = 1, \dots, s, \\
&\text{(c) } x_N = x_{N-1} + h\sum_{i=1}^{s} b_i K_i.
\end{aligned} \tag{34}$$

We propose the following half-explicit Runge–Kutta (HERK) method based on (34) for (1). The first stage-approximation $\Xi_1 = x_{N-1}$ is obviously available. The $(i+1)$ stage-approximation Ξ_{i+1} is obtained successively by solving the algebraic systems

$$\begin{aligned}
&\text{(a) } f\left(t_{N-1} + c_i h, \Xi_i, \frac{1}{a_{i+1,i}}\left[\frac{\Xi_{i+1} - x_{N-1}}{h} - \sum_{j=1}^{i-1} a_{i+1,j}K_j\right]\right) = 0, \\
&\text{(b) } g(t_{N-1} + c_{i+1}h, \Xi_{i+1}) = 0,
\end{aligned} \tag{35}$$

for $i = 1, \dots, s-1$. Finally, the numerical solution x_N at time step $t = t_N$ is determined by the system

$$\begin{aligned}
&\text{(a) } f\left(t_{N-1} + c_s h, \Xi_s, \frac{1}{b_s}\left[\frac{x_N - x_{N-1}}{h} - \sum_{i=1}^{s-1} b_i K_i\right]\right) = 0, \\
&\text{(b) } g(t_N, x_N) = 0.
\end{aligned} \tag{36}$$

Here

$$K_1 = \frac{\Xi_2 - x_{N-1}}{ha_{21}}, \qquad K_i = \frac{1}{a_{i+1,i}}\left[\frac{\Xi_{i+1} - x_{N-1}}{h} - \sum_{j=1}^{i-1} a_{i+1,j}K_j\right], \quad i = 2, \dots, s-1, \tag{37}$$

Table 1
Butcher tableau of explicit s-stage Runge–Kutta method .

$$\begin{array}{c|cccc} 0 & 0 & 0 & \cdots & 0 \\ c_2 & a_{2,1} & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ c_s & a_{s,1} & a_{s,2} & \cdots & 0 \\ \hline & b_1 & b_2 & \cdots & b_s \end{array}$$

and

$$K_s = \frac{1}{b_s}\left[\frac{x_N - x_{N-1}}{h} - \sum_{i=1}^{s-1} b_i K_i\right]. \tag{38}$$

Applying this method to the special matrix-valued DAE system (8), these become a system of linear matrix equations,

$$\begin{bmatrix} E_1(t_{N-1}^{(i)}) \\ A_2(t_{N-1}^{(i+1)}) \end{bmatrix} \Xi_{i+1} = \begin{bmatrix} E_1(t_{N-1}^{(i)}) \left[X_{N-1} + h\sum_{j=1}^{i-1} a_{i+1,j}K_j\right] + ha_{i+1,i}F(t_{N-1}^{(i)}, \Xi_i) \\ 0 \end{bmatrix},$$

for $i = 1, \ldots, s-1$, and

$$\begin{bmatrix} E_1(t_{N-1}^{(s)}) \\ A_2(t_N) \end{bmatrix} X_N = \begin{bmatrix} E_1(t_{N-1}^{(s)}) \left[X_{N-1} + h\sum_{i=1}^{s-1} b_i K_i\right] + hb_s F(t_{N-1}^{(s)}, X_s) \\ 0 \end{bmatrix},$$

respectively, where $t_{N-1}^{(i)} = t_{N-1} + c_i h$, $i = 1, \ldots, s$.

Again, when using direct solution methods, these linear systems can be solved efficiently by one LU factorization per system, i.e., a total of sLU factorizations is needed.

We now show that the HERK method (35)–(36) for (1) is exactly the HERK method analyzed in [12] applied to the equivalent semi-explicit index-2 DAE (7). Indeed, assume that now $f_{\dot{x}_1}$ is nonsingular and let $\Xi_i = (\Xi_{i,1}^T, \Xi_{i,2}^T)^T$ and $K_i = (K_{i,1}^T, K_{i,2}^T)^T$ be decomposed accordingly. Furthermore, assume that the approximation y_{N-1} to $y(t_{N-1})$ in (7) is the same as x_{N-1}. With new variables $Y_i = \Xi_i$ and $Z_i = K_{i,2}$, then we have $Y_1 = \Xi_1 = x_{N-1} = y_{N-1}$. Then, consider the system (35) with $i = 1$ for the next stage Ξ_2 and rewrite it using the new variables as follows:

$$\begin{aligned} &f(t_{N-1}, Y_{1,1}, Y_{1,2}, K_{1,1}, Z_1) = 0, \\ &K_{1,2} - Z_1 = 0, \\ &g(t_{N-1} + c_2 h, Y_2) = 0. \end{aligned}$$

By the definition of function φ and γ as in (7), we have the system

$$\begin{aligned} &K_1 = \varphi(t_{N-1}, Y_1, Z_1), \\ &0 = \gamma(t_{N-1} + c_2 h, Y_2), \end{aligned}$$

or equivalently by (37)

$$\begin{aligned} &Y_2 = y_{N-1} + ha_{2,1}\varphi(t_{N-1}, Y_1, Z_1), \\ &0 = \gamma(t_{N-1} + c_2 h, Y_2). \end{aligned}$$

Similarly, the system (35) with $i = 2$ for Ξ_3 is rewritten as

$$\begin{aligned} &f(t_{N-1} + c_2 h, Y_{2,1}, Y_{2,2}, K_{2,1}, Z_2) = 0, \\ &K_{2,2} - Z_2 = 0, \\ &g(t_{N-1} + c_3 h, Y_3) = 0, \end{aligned}$$

which reduces to

$$\begin{aligned} &K_2 = \varphi(t_{N-1} + c_2 h, Y_2, Z_2), \\ &0 = \gamma(t_{N-1} + c_3 h, Y_3). \end{aligned}$$

Using the definition of K_2 in (37) and inserting the preceding result $K_1 = \varphi(t_{N-1}, Y_1, Z_1)$, we obtain

$$\begin{aligned} &Y_3 = y_{N-1} + h\left(a_{3,1}\varphi(t_{N-1}, Y_1, Z_1) + a_{3,2}\varphi(t_{N-1} + c_2 h, Y_2, Z_2)\right), \\ &0 = \gamma(t_{N-1} + c_3 h, Y_3). \end{aligned}$$

By induction, we obtain

$$\begin{aligned}
&\text{(a)}\ Y_{i+1} = y_{N-1} + h\sum_{j=1}^{i} a_{i+1,j}\varphi(t_{N-1}^{(j)}, Y_j, Z_j),\\
&\text{(b)}\ 0 = \gamma(t_{N-1}^{(i+1)}, Y_{i+1}),
\end{aligned} \tag{39}$$

for $i = 1, \ldots, s-1$. Finally, the numerical solution y_N at time step $t = t_N$ is obtained by the system

$$\begin{aligned}
&\text{(a)}\ y_N = y_{N-1} + h\sum_{i=1}^{s} b_i\varphi(t_{N-1}^{(i)}, Y_i, Z_i),\\
&\text{(b)}\ 0 = \gamma(t_N, y_N).
\end{aligned} \tag{40}$$

Theorem 3 in [12] states that if the scheme (39)–(40) is consistent of order p, then it is convergent of order p. Furthermore, order conditions up to $p = 4$ are given in [12, Table 1]. For $p \le 2$, the order conditions are the same as in the ODE case. We thus immediately obtain the convergence result for the half-explicit Euler method and for the 2-stage half-explicit Runge–Kutta method (35)–(36).

Theorem 10. *Assume that the Runge–Kutta method given by Table 1 with $s = 2$ satisfies*

$$c_2 = a_{21}, \qquad b_1 + b_2 = 1, \qquad c_2 b_2 = 1/2. \tag{41}$$

If the initial condition x_0 is consistent, then the half-explicit Runge–Kutta (HERK) method (35)–(36) applied to (1) is convergent of order $p = 2$.

Proof. As we have just shown above, the scheme (35)–(36) is equivalent to the HERK method (39)–(40) that is analyzed in [12], and since conditions (41) are exactly the order conditions for $p = 2$ derived in [12, Table 1], the assertion follows directly from [12, Theorem 3]. □

Example 11. Explicit 2-stage Runge–Kutta methods satisfying (41) are given by a one-parameter family of methods as in the following Butcher tableau

$$\begin{array}{c|cc}
0 & 0 & 0\\
\alpha & \alpha & 0\\
\hline
 & 1-\frac{1}{2\alpha} & \frac{1}{2\alpha}
\end{array}$$

where $\alpha \in (0, 1]$ is a parameter. This class of methods is well-known to be of second order for ODEs. For $\alpha = 1/2$, we have the explicit midpoint rule, while for $\alpha = 1$, the explicit trapezoidal rule is obtained. The generalized stability function for the method as applied to the test DAE (22) is

$$R(z, w) = \frac{1}{1 + w(1-\alpha)}\left[1 + z + \frac{z^2}{2} + \alpha w\left(3 - 2\alpha + 2z(1+\alpha) - \alpha w(3 - 2\alpha) + \alpha z^2\right)\right].$$

For $w = 0$, the stability function $R(z) = 1 + z + z^2/2$ is exactly the stability function of the explicit Runge–Kutta method (11) that is well analyzed in the numerical analysis of non-stiff ODEs, see e.g. [8].

One might think that the construction of high-order HERKs is similar to the ODE case. However, as pointed out in [25,12], for order $p \ge 3$, extra order conditions must be fulfilled in addition to those for ODEs. It is shown there as well that there exists only one HERK method with $p = s = 3$ and no method of order $p = 4$ with $s = 4$. In [25,12], HERK methods of order $p = 4$ and $p = 5$ are constructed with the number of stages $s = 5$ and $s = 8$, respectively. They can obviously be adopted in (35)–(36) with the same convergence order. In [10,13], a modification of the HERK methods for index-2 DAEs is proposed which makes high-order methods available with lower stage-number. However, this version of HERK methods would require the initial value for the artificial algebraic variable $z(0) = \dot{x}_2(0)$ (using again a splitting into algebraic and differential variables), which does not seem to be natural in the context of our original problem (1).

Remark 12. The half-explicit Runge–Kutta methods proposed here for strangeness-free DAEs (1) can be considered as a generalization of the half-explicit Runge–Kutta methods for semi-explicit index-1 DAEs analyzed in [11,3]. However, their implementations and convergence results are different. For semi-explicit DAEs, not only the differential and the algebraic parts are separated, but also the derivative of the differential component is explicitly given, which is not the case with (1). Hence, the differential component of each stage is computed first and then the algebraic component follows by solving an algebraic system. Here, the whole stage-approximation must be evaluated once by solving a larger algebraic system. In fact, in the case of semi-explicit systems, we have $\partial f/\partial \dot{x} = E_1 = \begin{bmatrix} I & 0 \end{bmatrix}$, hence the Jacobian of the algebraic system (35) has a special lower block-triangular form with the identity matrix in the left upper block. This special structure makes the use of half-explicit Runge–Kutta methods simpler when they are applied to semi-explicit DAEs of index 1.

Table 2
Actual errors of solutions to IVP (42) by one-leg Adams–Bashforth method in Example 5.

ξ	h	Error in x_1	Error order in x_1	Error in x_2	Error order in x_2
2	0.1	0.004791028	2.17	0.001762521	2.17
2	0.05	0.001067391	2.10	0.000392671	2.10
2	0.025	0.00024866	2.06	9.14768E−05	2.06
2	0.01	3.79341E−05	2.02	1.39552E−05	2.02
2	0.005	9.32463E−06	2.01	3.43034E−06	2.01
2	0.0025	2.31107E−06	2.01	8.50196E−07	2.01
1.5	0.1	0.005075127	2.25	0.001867035	2.25
1.5	0.05	0.001069938	2.16	0.000393608	2.16
1.5	0.025	0.000239792	2.09	8.82147E−05	2.09
1.5	0.01	3.55486E−05	2.04	1.30776E−05	2.04
1.5	0.005	8.64526E−06	2.02	3.18041E−06	2.02
1.5	0.0025	2.13074E−06	2.01	7.83855E−07	2.01
1	0.1	0.004108619	2.64	0.001511476	2.64
1	0.05	0.000657134	2.54	0.000241746	2.54
1	0.025	0.000112741	2.40	4.14753E−05	2.40
1	0.01	1.27928E−05	2.22	4.7062E−06	2.22
1	0.005	2.74791E−06	2.12	1.0109E−06	2.12
1	0.0025	6.30058E−07	2.07	2.31785E−07	2.07
0.5	0.1	0.004996419	0.73	0.00183808	0.73
0.5	0.05	0.003007934	1.57	0.001106557	1.57
0.5	0.025	0.001016036	1.81	0.000373779	1.81
0.5	0.01	0.000190678	1.93	7.01463E−05	1.93
0.5	0.005	5.01435E−05	1.96	1.84468E−05	1.96
0.5	0.0025	1.28518E−05	1.98	4.72791E−06	1.98

Table 3
Actual errors of solutions to IVP (42) by half-explicit Runge–Kutta method in Example 11.

α	h	Error in x_1	Error order in x_1	Error in x_2	Error order in x_2
1	0.1	0.009389536	1.96	0.003454217	1.96
1	0.05	0.002411295	1.98	0.000887066	1.98
1	0.025	0.000610229	1.99	0.000224491	1.99
1	0.01	9.83115E−05	2.00	3.61668E−05	2.00
1	0.005	2.46325E−05	2.00	9.06178E−06	2.00
1	0.0025	6.16487E−06	2.00	2.26793E−06	2.00
0.5	0.1	0.004037535	1.96	0.001485326	1.96
0.5	0.05	0.00103773	1.98	0.000381759	1.98
0.5	0.025	0.000262811	1.99	9.66827E−05	1.99
0.5	0.01	4.23638E−05	2.00	1.55848E−05	2.00
0.5	0.005	1.06166E−05	2.00	3.90564E−06	2.00
0.5	0.0025	2.65735E−06	2.00	9.77584E−07	2.00

5. Numerical experiments

Half-explicit methods as derived in the preceding sections have been implemented and applied to DAE examples. For illustration we present results for the half-explicit versions of the one-leg Adams–Bashforth method (HEOL) from Example 5, the two-step Adams–Bashforth method (HEAB) from Example 8, and the trapezoidal and midpoint Runge–Kutta methods (HETRA, HEMID) from Example 11.

Example 13. Our first test problem is an artificially constructed DAE with a known exact solution. We consider the DAE

$$\begin{bmatrix} 1 & t \\ 0 & 0 \end{bmatrix} \dot{x} = \begin{bmatrix} x_1 x_2 + e^t + t\cos t - e^t \sin t \\ e^{-t} x_1 - x_2 + \sin t - 1 \end{bmatrix}, \quad 0 \le t \le 1, \tag{42}$$

together with the initial condition $x(0) = [0, 1]^T$. It is easy to check that the DAE is strangeness-free and that the exact unique solution is $x_1 = e^t$, $x_2 = \sin t$. We have solved the initial value problem by the described HEOL and HERK methods on a uniform mesh with different stepsize h. The actual errors $\max |x_i(t_N) - x_{i,N}|$, $i = 1, 2$, of different methods versus h are displayed in Tables 2 and 3. In addition, based on the actual errors, we also give numerical estimates for the convergence rate, which confirm the proved convergence orders.

Example 14. We have also tested the presented methods for matrix-valued DAEs of type (8), see [21] for tables of performance results, which demonstrate that the methods produce numerical results of almost the same accuracy as fully implicit methods but require much less CPU time.

6. Conclusion

We have discussed the use of half-explicit methods for solving general nonlinear DAEs in strangeness-free form. Half-explicit variants of explicit one-leg, linear multistep, and Runge–Kutta methods have been proposed and analyzed. These classes of methods are more efficient in solving non-stiff DAEs than the common implicit methods like BDF and Radau5. A particular advantage of these methods arises in the solution of some semi-linear matrix-valued DAEs systems arising in the numerical computation of Lyapunov spectral intervals.

We have shown that for strangeness-free DAEs of the form (1) half-explicit one-leg methods behave like BDF methods, while for half-explicit multistep methods and Runge–Kutta methods the situation is rather similar to the analysis for semi-explicit index-2 DAEs. Either extra stability condition or extra order conditions are required.

Finally, we comment on two problems which are worth being investigated in the future. First, it would be interesting to appropriately adapt the high-order HERK methods in [10,13] to (1). Second, the classes of half-explicit methods discussed in this paper are suitable for non-stiff DAEs. However, many DAEs arising in applications are stiff. For strangeness-free stiff DAEs, the half-explicit framework can be combined with Runge–Kutta–Chebyshev methods, which are explicit methods and known to efficiently solve stiff ODEs [26]. A complete analysis of half-explicit Runge–Kutta–Chebyshev methods for stiff DAEs of the form (1) is also of great interest with respect to many applications in solving semi-discretized partial differential(-algebraic) equations.

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