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Semi-Lagrangian multistep exponential integrators for index 2 differential–algebraic systems

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ABSTRACT

Implicit-explicit (IMEX) multistep methods are very useful for the time discretization of convection diffusion PDE problems such as the Burgers equations and the incompressible Navier–Stokes equations. In the latter as well as in PDE models of plasma physics and of electromechanical systems, semi-discretization in space gives rise to differential–algebraic (DAE) system of equations often of index higher than 1. In this paper we propose a new class of exponential integrators for index 2 DAEs arising from the semi-discretization of PDEs with a dominating and typically nonlinear convection term. This class of problems includes the incompressible Navier–Stokes equations. The integration methods are based on the backward differentiation formulae (BDF) and they can be applied without modifications in the semi-Lagrangian integration of convection diffusion problems. The approach gives improved performance at low viscosity regimes.

1. Introduction

We consider differential–algebraic equations (DAEs) of the form

$$\begin{aligned} \dot{y} &= C(y)y + f(y,z), \\ 0 &= g(y), \end{aligned} \tag{1}$$

with consistent initial data $y(t_0) = y_0$, $z(t_0) = z_0$, where $y = y(t) \in \mathbb{R}^n, z = z(t) \in \mathbb{R}^m$, for all $t \in [t_0, T]$; while $f : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^n, g : \mathbb{R}^n \to \mathbb{R}^m$, and $C = C(y) : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ is a matrix-valued function of y. The notation $\dot{y}$ denotes the derivative with respect to t. DAEs of this type arise, for example, from the semi-discretization (in space) of PDE models in plasma physics, and also of the incompressible Navier–Stokes equations. In this case $C(y)y$ represents the nonlinear convection term, $f(y,z)$ represents the diffusion and pressure terms and $g(y)$ comes from the incompressibility constraint; f and g are both linear in this case. Assuming (1) generally results from a convection diffusion PDE, we will refer to the term $C(y)y$ as the convecting vector field or simply the convection term.

The system of DAEs (1) is of *differential index* 2 if the functions f, g are sufficiently differentiable and the matrix $g_y f_z$ is non-singular in a neighbourhood of the solution. Here f_z and g_y denote Jacobian transformations of f and g The algebraic part of (1) represents the main constraint. A second (hidden) constraint,

$$g_y(y)(C(y)y + f(y,z)) = 0, \tag{2}$$

is given by differentiating the main algebraic constraint with respect to t. The variable y is commonly referred to as the *differential or state* variable while the z-variable is the *algebraic or constraint* variable or simply the *Lagrange multiplier*. For more details about index 2 DAEs we refer to [1] for example.

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Runge–Kutta (RK) methods have been considered for the time discretization of index 2 DAE systems (see [2–4,1,5,6]). Some of these RK methods achieve high order of convergence with comparatively little storage requirements and have good stability properties. However, fully implicit RK methods generally have a drawback over the *IMEX*[1] or *DIRK*.[2] methods in terms of computational costs per time step. For reasons of ease of implementation, we only wish to consider IMEX methods, whereby we treat the nonlinear term $C(y)y$ explicitly and the term $f(y,z)$ implicitly as it may be stiff and linear in some applications.

One-step IMEX methods for hyperbolic systems with relaxation have recently been studied in [7] and applied to index-1 DAEs in [8]. In the framework of IMEX one-step exponential integrators, we have earlier considered *DIRK-CF* methods for convection diffusion PDE problems [9]. These methods are based on commutator-free[3] (CF) Lie group methods and are typically constructed from IMEX RK methods where the implicit part is a DIRK method (see Appendix A.3 for details on IMEX-CF exponential integrators and DIRK-CF methods in particular). The main reason for developing this type of methods is that they can be applied to the semi-Lagrangian numerical integration of convection diffusion PDEs, achieving improved stability behavior in the small viscosity limit.

When applied directly to problems of the type (1), the DIRK-CF methods can however only give convergence of order 2. The same remains true when using IMEX RK methods such as those in [11,12]. DIRK methods for (1) may appear cheaper to implement than fully implicit RK methods, but the order of convergence is greatly limited by the stage order.[4] For example the DIRK methods with nonzero diagonal entries, e.g. most of the methods in [13,11], will give convergence of order at most 2 (see [2, p.18] and [1, Lemma 4.4, Thm. 4.5, p.495–496]). All the DIRK methods in [12,14,15] have stage order at most 2, thus they would lead to convergence of order at most 3 (according to [16, Thm.5.2]).

On the other hand, linear k-step methods such as BDF methods, are known to give convergence of order $p = k$, for $1 \leqslant k \leqslant 6$, in both variables (see for example [1, VII.3]). They are also known to be A-stable for $1 \leqslant k \leqslant 2$ and $A(\alpha)$-stable for $3 \leqslant k \leqslant 6$. We however do not wish to treat the whole system implicitly. IMEX multistep methods based on BDF schemes have been developed and applied for the time discretization of convection diffusion PDE problems such as the Burgers equations (see for example [17]) as well as the incompressible Navier–Stokes equations (see [18–23]).

We hereby propose a new class of exponential integrators for (1) based on the backward differentiation formula (BDF). We name these methods *BDF-CF* for short. They have about the same implementation ease as the DIRK-CF, and as such they can be regarded as their multistep counterpart. Their main advantage compared to the DIRK-CF is that they can achieve order of convergence higher than 2, when applied to (1) both in the algebraic and differential variables.

The methods are a subclass of the IMEX multistep methods and they are closely related to the SBDF methods presented and studied in [17,24]. Compared to these methods the BDF-CF methods can be used without modifications in a semi-Lagrangian approach to convection diffusion problems, whereby the exponentials must be realized as flows of pure convection problems. The pure convection flows are typically implemented by tracing characteristics, as in [9,22,25], or by computing more accurate approximations of the pure convection flows as in [18,26] (this can for example be achieved using an integration method of higher order).

We recall that the concept of multistep exponential integrators is not new to this paper. Explicit multistep exponential integrators have recently been studied for semilinear ODEs with a linear stiff term and a nonlinear non stiff term, see [27–29]. These methods require the computation of exponentials of the linear stiff term, and the obtained schemes are fully explicit. If the nonlinear term represents convection and is in the form $C(y)y$, the methods we present here can also be applied to such ODEs, but our assumption is that the problems are convection dominated and therefore we treat the nonlinear term explicitly by exponentials (or accurate solution of pure convection flows) and the linear term implicitly. Commutator-free methods of multistep type were originally considered in [30].

1.1. The BDF-CF methods

We define the k-step exponential BDF (or simply BDF-CF) method as follows: Given k initial values $y_0,\ldots,y_{k-1}$, find (y_k,z_k) such that

$$\begin{aligned} \alpha_k y_k + \sum_{i=0}^{k-1} \alpha_i \varphi_i y_i &= hf(y_k, z_k), \\ 0 &= g(y_k), \end{aligned} \tag{3}$$

where $\varphi_i := \exp(\sum_{j=0}^{k-1} a_{i+1,j+1} hC(y_j)),\ i = 0,\ldots,k-1$, and $a_{ij} \in \mathbb{R},\ i,j = 1,\ldots,k$, are coefficients of the method, while α_i, $i = 0,\ldots,k$, are coefficients of the linear k-step classical BDF method. The use of the functions φ_i (exact flows of the linearized convection term) is introduced to obtain improved performance in the treatment of convection dominated problems. This idea was also found useful in the DIRK-CF methods [9] and in the multirate methods for atmospheric flow simulation

[1] *Implicit-explicit* (IMEX): Methods that treat, for example, the term $C(y)y$ explicitly and the remaining terms implicitly.
[2] *Diagonally implicit RK* (DIRK): Implicit RK method with coefficients $\{a_{ij}\}$ such that $a_{ij} = 0$ for all $i < j$.
[3] Using the terminology of [10]. See also Appendix A.3 for further details.
[4] A RK method with coefficients $\{a_{ij}, b_i, c_i\}$, $i, j = 1,\ldots,s$, has (internal) *stage order* q, if q is the greatest integer such that $\sum_{j=1}^{s} a_{ij} c_j^{k-1} = c_i^k/k,\ i = 1,\ldots,s$ hold for all $k = 1,\ldots,q$.