NORGES TEKNISK-NATURVITENSKAPELIGE UNIVERSITET

Semi-Lagrangian multistep exponential integrators for index 2 differential algebraic system

by

Bawfeh Kingsley Kometa and Elena Celledoni

PREPRINT
NUMERICS NO. 3/2010

NORWEGIAN UNIVERSITY OF
SCIENCE AND TECHNOLOGY
TRONDHEIM, NORWAY

This report has URL `http://www.math.ntnu.no/preprint/numerics/2010/N3-2010.pdf`
Address: Department of Mathematical Sciences, Norwegian University of Science and Technology, N-7491 Trondheim, Norway.

Semi-Lagrangian multistep exponential integrators for index 2 differential algebraic system

Bawfeh Kingsley Kometa and Elena Celledoni

May 19, 2010

Implicit-explicit (IMEX) multistep methods are very useful for the time discretization of convection diffusion PDE problems such as the Burgers equations and also the incompressible Navier-Stokes equations. Semi-discretization in space of the latter typically gives rise to an index 2 differential- algebraic (DAE) system of equations. Runge-Kutta (RK) methods have been considered for the time discretization of such DAE systems. However, due to their implicit nature, they generally have a drawback over the IMEX multistep methods in terms of computational costs per step. In this paper we propose an exponential integration method for index 2 DAEs of a special class that includes the type arising from the incompressible Navier-Stokes problem. The methods are based on the backward differentiation formulae (BDF), belong to the class of IMEX multistep methods and are unconditionally stable.

Keywords: index 2 DAEs, exponential integrators, IMEX multistep, BDF.

1 Introduction

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

$$\dot{y} = C(y)y + f(y,z), \tag{1.1a}$$
$$0 = g(y), \tag{1.1b}$$

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 also arise from the semi-discretization (in space) of the incompressible Navier-Stokes equations, where $C(y)y$ represents the nonlinear convection term, $f(y,z)$ represents the diffusion and pressure terms and $g(y)$ comes from the incompressibility constraint. Assuming (1.1) generally result 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 (1.1) is of *differential index* 2 if the functions f, g are sufficiently differentiable and the matrix $f_z g_y$ is nonsingular in a neighbourhood of the solution. The algebraic part (1.1b) represents the main constraint. A second (hidden) constraint,

$$g_y(y)(C(y)y + f(y,z)) = 0, \tag{1.2}$$

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.*

Runge-Kutta (RK) methods have been considered for the time discretization of index 2 DAE systems (see [10, 9, 2, 21, 15, 16]). Some of these RK methods achieve high order of convergence with comparatively little storage requirements and have good stability properties. However, due to their implicit nature, they generally have a drawback over the IMEX[1] multistep methods in terms of computational costs per time step. For reasons of ease of implementation, we only wish to consider IMEX methods that treat the nonlinear term $C(y)y$ explicitly and the term $f(y,z)$ implicitly as it may be stiff and linear in most applications.

Among the class of implicit RK (IRK) methods, DIRK[2] methods applied to (1.1) appear cheaper to implement than fully implicit RK methods. DIRK methods require solving at most one linear system per stage, for example, if (1.1) is linear. However, the order of convergence is greatly limited by the stage order[3] of the DIRK methods (which is at most 3 for most of the DIRK methods in the literature). For example the DIRK methods with nonzero diagonal entries, e.g. most of the methods in [1, 3], will give convergence of order at most 2 (see [9, p.18] and [10, Lemma4.4, Thm.4.5, p.495-496]). All the DIRK methods in [19, 25, 20] have stage order at most 3, thus they would lead to convergence of order at most 3 (according to [14, Thm.5.2]).

In the framework of exponential integrators, we have considered a direct application of the Lie group methods proposed by the authors in [7] to solve (1.1). These methods are typically constructed from IMEX partitioned RK methods with a DIRK part, and are referred to as *DIRK-CF* (See Appendix A.3 for details). Without much surprise we found that the DIRK-CF methods (constructed from various IMEX RK methods with DIRK parts) only give convergence of order 2, since both the stage orders of the DIRK and explicit RK (ERK) methods are low. We obtain a similar observation with direct application of various IMEX RK methods (with DIRK parts) such as those in [3] and [19].

Linear k-step BDF methods, on the other hand, are known to give convergence of order $p = k$, for $1 \leqslant k \leqslant 6$, in both variables (see for example [10, VII.3]). The BDF methods are 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 nonlinear term $C(y)y$ implicitly. IMEX multistep methods have been developed and applied for the time discretization of convection diffusion PDE problems such as the Burgers equations (see for example [18, 4]) and also the incompressible Navier-Stokes equations (see [22, 17, 12, 24, 28, 8]). Semi-discretization in space of the latter typically gives rise to an index 2 differential- algebraic (DAE) system of the type (1.1). We hereby propose a new class of exponential integrators for (1.1) which are multistep and based on the backward differentiation formula (BDF). We name these methods *BDF-CF* for short. The methods are a subclass of IMEX multistep methods and has about the same implementation ease as the DIRK-CF but can give us order of convergence higher than 2 both in the algebraic and differential variables. We recall that explicit multistep exponential integrators have recently been studied for semilinear ODEs by Calvo and Palencia [5] and also by Ostermann and Thalhammer [23]. There the authors consider exponentials of the linear term. The methods we present here can also be applied to such ODEs (if we can express the nonlinear term in the form $C(y)y$), but we would treat the nonlinear term explicitly by exponentials and the linear term implicitly.

Hence given k initial values $y_0, \ldots, y_{k-1}$, we define the k-step exponential BDF (BDF-CF)

[1]IMEX methods are time integration methods that treat, for example, the term $C(y)y$ explicitly and the remaining terms implicitly.

[2]A RK method with coefficients $\{a_{ij}, b_i, c_i\}$, $i, j = 1, \ldots, s$, is called *diagonally implicit* or *DIRK* if $a_{ij} = 0$ for all $i > j$ and $a_{ii} \neq 0$ for some $i = 1, \ldots, s$.

[3]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 $\sum_{j=1}^{s} a_{ij} c_j^{k-1} = c_i^k / k, \quad i = 1, \ldots, s$ hold for all $k = 1, \ldots, q$.

method as follows: Find (y_k, z_k) such that

$$\begin{aligned} \alpha_k y_k + \sum_{i=0}^{k-1} \alpha_i \varphi_i y_i &= h f(y_k, z_k), && (1.3a) \\ 0 &= g(y_k) && (1.3b) \end{aligned}$$

where $\varphi_i := \exp\left(\sum_{j=0}^{k-1} a_{i+1,j+1} hC(y_j)\right)$, $i = 0, \ldots, k-1$, 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. Methods of this type permit the exact integration of the convection term via exponentials, an idea also found useful in the DIRK-CF methods for convection dominated convection diffusion PDEs [7] and in the multirate methods for atmospheric flow simulation [27]. We refer to this kind of methods as *commutator-free*[4] (CF) multistep exponential integrators, since they involve matrix exponentials whose exponents do not contain matrix commutators. Thus the name BDF-CF is used for the method (1.3). In a more general setting involving CF exponential integrators [6], the functions φ_i would be defined as a composition of matrix exponentials. However, in the BDF-CF methods considered here single exponentials would suffice. More precisely we shall write a k-order (typically k-step) method as BDFk-CF. The overall method is termed *semi-Lagrangian* if we treat each flow, $\varphi_i y_i$, in a semi-Lagrangian fashion (described in [7, Sect.3.1]), and is found useful for the time integration of convection diffusion PDEs and the Navier-Stokes equations. Nevertheless, the flows can also be computed using other numerical methods such as the direct approximation of the matrix exponentials via a Padé approximant or by using a Krylov subspace method. The semi-Lagrangian approach was shown [7] to be more stable and accurate than the latter two methods, in the solution of convection dominated convection-diffusion problems. A further requirement in the semi-Lagrangian case is to have the matrix-valued function $C(y)$ *linear*. In this paper the semi-Lagrangian approach has been used in all numerical experiments involving time dependent PDEs.

Assuming once again that the system (1.1) arises from the semi-discretization (in space) of a PDE (e.g.,the Navier-Stokes equations), then a close comparison of the BDF-CF methods with the operator-integrating-factor splitting methods of Maday *et al.* [22] (also considered in [8]) will be as follows: Find (y_k, z_k) such that

$$\alpha_k y_k + \sum_{i=0}^{k-1} \alpha_i \tilde{y}_i = h f(y_k, z_k), \quad g(y_k) = 0, \tag{1.4}$$

where α_i are coefficients of the classical $k-$step BDF method, and $\tilde{y}_i$ are solutions of linearized pure convection problems

$$\dot{\tilde{y}} = C(p_k(t))\tilde{y}, \quad t \in (t_i, t_k), \quad \tilde{y}(t_i) = y_i$$

where $p_k(t) \in \mathbb{R}^n$ is a $(k-1)$-degree polynomial extrapolation of the initial values. The BDF-CF methods, however, compute the values $\tilde{y}_i := \varphi_i y_i$ in a different manner (without a special linearization of the convection term).

The rest of the paper is organized as follows. In Section 2 we present a derivation of the new class of methods. In Section 3 we state some convergence results for the methods and provide a numerical evidence for the convergence of methods up to order 4. We discuss the stability of the methods in Section 4, making comparisons with some well-known IMEX multistep methods in the literature. Unless stated otherwise, we shall say that a method has *'order' p* to refer to the temporal order of convergence of the method. Also we shall only consider constant time steps,

[4]using the terminology of Celledoni *et al.* [6]

which shall be written as $h := \Delta t$. Given initial time t_0, we shall write t_n to denote time level n such that $t_n := t_0 + nh$. For a given field variable $v = v(t)$ we denote the numerical approximation at time t_n by $v_n \approx v(t_n)$. In general we shall use the notation $\|\cdot\|$ for an arbitrary but well-defined norm of a vector or function.

2 Construction of commutator-free exponential BDF methods

Given a discrete time interval $t_0, \ldots, t_K = T$ and initial data $y_0, \ldots, y_{k-1}$, $1 \leqslant k \leqslant K$, we describe a $k-$step BDF-CF method as follows

---

Algorithm 1. *BDF-CF method*

---

for $n = k-1$ ***to*** $K-1$ ***do***

$$\begin{aligned} \varphi_i &= \exp\left(h\sum_{j=1}^{k} a_{i+1,j} C(y_{n-k+j})\right), \quad i = 0, \ldots, k-1, \\ \alpha_k y_{n+1} + \sum_{i=0}^{k-1} \alpha_i \varphi_i y_{n+1-k+i} &= hf(y_{n+1}, z_{n+1}), \qquad (2.1a) \\ 0 &= g(y_{n+1}) \qquad (2.1b) \end{aligned}$$

end for

---

where $a_{i,j} \in \mathbb{R}$, $i, j = 1, \ldots, k$, are coefficients of the BDF-CF method and α_i are coefficients of the classical $k-$step BDF method. Thus one can represent a $k-$step BDF-CF method in terms of its coefficients as in the following table

$$\begin{array}{c|ccc} y_{n-k+1} & a_{1,1} & \ldots & a_{1,k} \\ \vdots & \vdots & \ldots & \vdots \\ y_n & a_{k,1} & \ldots & a_{k,k} \\ \hline & C(y_{n-k+1}) & \ldots & C(y_n) \end{array}$$

So that for each $n \geqslant k-1$ the method solves for the unknown values, y_{n+1}, z_{n+1}, given the initial values $y_{n-k+1}, \ldots, y_n$. For reasons of convenience (but without loss of generality) we shall often drop the index n or simply treat the case with $n = k-1$ as in (1.3). The first order (one-step) BDF-CF method is simply the semi-explicit backward Euler method, obtained by choosing $\varphi_0 = \exp(hC(y_n))$ in (1.3). We shall therefore only consider k-step methods, for $k \geqslant 2$.

For simplicity we shall restrict the analysis of the methods to an ODE of the form

$$\dot{y} = C(y)y + f(y). \qquad (2.2)$$

Extension to the DAE (1.1) is more or less direct.

Let us denote the exact value at time t_j by $\hat{y}_j := y(t_j)$, $\quad j = 0, \ldots k$, and write $\hat{\varphi}_i := \exp\left(h\sum_{j=0}^{k-1} a_{i+1,j+1} C(y(t_j))\right)$, $\quad i = 0, \ldots, k-1$. Also let $\dot{\hat{y}}_j$, $\ddot{\hat{y}}_j, \ldots$ denote the derivatives with respect to the time variable.

2.1 Second order method (BDF2-CF)

The *truncation error* $\tau_2(h)$ for a two-step method is given by

$$\frac{1}{h}\left[\frac{3}{2}\hat{y}_2 - 2\hat{\varphi}_1\hat{y}_1 + \frac{1}{2}\hat{\varphi}_0\hat{y}_0\right] = f(\hat{y}_2) + \tau_2(h). \tag{2.3}$$

For a classical second order BDF method we have

$$\frac{1}{h}\left[\frac{3}{2}\hat{y}_2 - 2\hat{y}_1 + \frac{1}{2}\hat{y}_0\right] = C(\hat{y}_2)\hat{y}_2 + f(\hat{y}_2) + O(h^2). \tag{2.4}$$

For a second order method $\tau_2(h) = O(h^2)$. Therefore combining (2.3) and (2.4) will give

$$\frac{1}{h}\left[2\hat{\varphi}_1\hat{y}_1 - \frac{1}{2}\hat{\varphi}_0\hat{y}_0 - 2\hat{y}_1 + \frac{1}{2}\hat{y}_0\right] - C(\hat{y}_2)\hat{y}_2 = O(h^2), \tag{2.5}$$

which is a reasonable requirement for a second order method.

Putting

$$\begin{aligned}\hat{y}_0 &= \hat{y}_1 - h\dot{\hat{y}}_1 + O(h^2),\\ \hat{y}_2 &= \hat{y}_1 + h\dot{\hat{y}}_1 + O(h^2),\end{aligned}$$

we get via Taylor expansion (about $t = t_1$)

$$\begin{aligned}C(\hat{y}_2)\hat{y}_2 &= C(\hat{y}_1)\hat{y}_1 + hC(\hat{y}_1)\dot{\hat{y}}_1 + hC'(\hat{y}_1)(\dot{\hat{y}}_1)\hat{y}_1 + O(h^2),\\ \hat{\varphi}_0\hat{y}_0 &= \hat{y}_0 + a_{11}h[C(\hat{y}_1) - hC'(\hat{y}_1)(\dot{\hat{y}}_1)](\hat{y}_1 + h\dot{\hat{y}}_1) + a_{12}hC(\hat{y}_1)(\hat{y}_1 + h\dot{\hat{y}}_1)\\ &\quad + \frac{h^2}{2}(a_{11} + a_{12})^2 C^2(\hat{y}_1)\hat{y}_1 + O(h^3),\\ \hat{\varphi}_1\hat{y}_1 &= \hat{y}_1 + a_{21}h[C(\hat{y}_1) - hC'(\hat{y}_1)(\dot{\hat{y}}_1)]\hat{y}_1 + a_{22}hC(\hat{y}_1)\hat{y}_1 + \frac{h^2}{2}(a_{21} + a_{22})^2 C^2(\hat{y}_1)\hat{y}_1 + O(h^3).\end{aligned}$$

Substituting into (2.5) and comparing coefficients of like terms and powers of h we obtain the following order conditions on the coefficients for order 2

$$\begin{aligned}2(a_{21} + a_{22}) - \frac{1}{2}(a_{11} + a_{12}) - 1 &= 0, &\text{(2.6a)}\\ -2a_{21} + \frac{1}{2}a_{11} - 1 &= 0, &\text{(2.6b)}\\ \frac{1}{2}(a_{11} + a_{12}) - 1 &= 0, &\text{(2.6c)}\\ (a_{21} + a_{22})^2 - \frac{1}{4}(a_{11} + a_{12})^2 &= 0. &\text{(2.6d)}\end{aligned}$$

Solving this system yields a one-parameter set of coefficients, illustrated in the following table

y_{n-1}	$2(1 + 2\gamma)$	-4γ
y_n	γ	$1 - \gamma$
	$C(y_{n-1})$	$C(y_n)$

from which we define the second order BDF2-CF methods as

$$\frac{3}{2}y_{n+1} - 2\varphi_1 y_n + \frac{1}{2}\varphi_0 y_{n-1} = hf(y_{n+1}), \quad n \geqslant 1, \tag{2.7}$$

where $\varphi_0 = \exp\left(2(1+\gamma)hC(y_{n-1}) - 4\gamma hC(y_n)\right)$, and $\varphi_1 = \exp\left(\gamma hC(y_{n-1}) + (1-\gamma)hC(y_n)\right)$. Applied to the DAE (1.1) we get

$$\begin{aligned} \frac{1}{h}[\frac{3}{2}y_{n+1} - 2\varphi_1 y_n + \frac{1}{2}\varphi_0 y_{n-1}] &= f(y_{n+1}, z_{n+1}), \\ 0 &= g(y_{n+1}). \end{aligned} \tag{2.8}$$

2.2 Third order method (BDF3-CF)

The truncation error $\tau_3(h)$ for a three-step method is given by

$$\frac{1}{h}\left[\frac{11}{6}\hat{y}_3 - 3\hat{\varphi}_2\hat{y}_2 + \frac{3}{2}\hat{\varphi}_1\hat{y}_1 - \frac{1}{3}\hat{\varphi}_0\hat{y}_0\right] = f(\hat{y}_3) + \tau_3(h). \tag{2.9}$$

A classical third order BDF method will satisfy

$$\frac{1}{h}\left[\frac{11}{6}\hat{y}_3 - 3\hat{y}_2 + \frac{3}{2}\hat{y}_1 - \frac{1}{3}\hat{y}_0\right] = C(\hat{y}_3)\hat{y}_3 + f(\hat{y}_3) + O(h^3). \tag{2.10}$$

Combining (2.9) and (2.10), and requiring that $\tau_3(h) = O(h^3)$ we get

$$\frac{1}{h}\left[3\hat{\varphi}_2\hat{y}_2 - \frac{3}{2}\hat{\varphi}_1\hat{y}_1 + \frac{1}{3}\hat{\varphi}_0\hat{y}_0 - 3\hat{y}_2 + \frac{3}{2}\hat{y}_1 - \frac{1}{3}\hat{y}_0\right] - C(\hat{y}_3)\hat{y}_3 = O(h^3). \tag{2.11}$$

We put in (2.11)

$$\begin{aligned} \hat{y}_0 &= \hat{y}_1 - h\dot{\hat{y}}_1 + \frac{h^2}{2}\ddot{\hat{y}}_1 + O(h^3), \\ \hat{y}_2 &= \hat{y}_1 + h\dot{\hat{y}}_1 + \frac{h^2}{2}\ddot{\hat{y}}_1 + O(h^3), \\ \hat{y}_3 &= \hat{y}_1 + 2h\dot{\hat{y}}_1 + 2h^2\ddot{\hat{y}}_1 + O(h^3), \end{aligned}$$

and carry out a Taylor expansion (about $t = t_1$). Comparing coefficients of like terms and powers of h we obtain the order conditions for order 3, comprising of 10 linearly dependent equations in 9 unknowns (see Appendix A.2). Solving the system of equations in Maple yields a three-parameter family of methods, illustrated in the following table

$$\begin{array}{c|ccc} y_{n-2} & \frac{33}{2} - \frac{9}{4}\beta - 9\gamma & -18 + 9\alpha + \frac{9}{2}\beta + 9\gamma & \frac{9}{2} - 9\alpha - \frac{9}{4}\beta \\ y_{n-1} & 3 + 2\alpha - \frac{1}{2}\beta - 2\gamma & \beta & -1 - 2\alpha - \frac{1}{2}\beta + 2\gamma \\ y_n & \alpha & 1 - \alpha - \gamma & \gamma \\ \hline & C(y_{n-2}) & C(y_{n-1}) & C(y_n) \end{array},$$

from which the third order BDF3-CF methods are defined for $n \geqslant 2$.

2.3 Fourth order method (BDF4-CF)

We determine the coefficients, $\{a_{ij}\}$, $i, j = 1, \ldots, 4$, for the fourth order method by requiring that the equation

$$\frac{1}{h}\left[4\hat{\varphi}_3\hat{y}_3 - 3\hat{\varphi}_2\hat{y}_2 + \frac{4}{3}\hat{\varphi}_1\hat{y}_1 - \frac{1}{4}\hat{\varphi}_0\hat{y}_0 - 4\hat{y}_3 + 3\hat{y}_2 - \frac{4}{3}\hat{y}_1 + \frac{1}{4}\hat{y}_0\right] - C(\hat{y}_4)\hat{y}_4 = O(h^4) \tag{2.12}$$

is satisfied. Again using Taylor expansion and comparing coefficients of like terms we obtain a 6-parameter set of coefficients given by

$$
\begin{array}{c|cc}
y_{n-3} & 4\alpha - 4\sigma - 8\varrho + 12 + \gamma + 2\kappa & -4\alpha + 8\varrho - 2\gamma - 3\kappa - 8 + 4\sigma \\
y_{n-2} & -3\beta + 3\alpha - \frac{3}{2}\varrho + \frac{3}{16}\gamma + \frac{3}{8}\kappa - \frac{3}{4}\sigma + \frac{3}{2} & 9\beta - \frac{9}{2}\alpha - \frac{9}{8}\varrho - \frac{9}{32}\gamma - \frac{9}{32}\kappa - \frac{9}{8}\sigma + \frac{21}{4} \\
y_{n-1} & \alpha & 2 - \varrho - \sigma - \alpha \\
y_n & \beta & \frac{1}{4} - 3\beta + \frac{1}{2}\alpha + \frac{1}{8}\varrho - \frac{3}{32}\kappa - \frac{1}{32}\gamma - \frac{1}{8}\sigma \\
\hline
 & C(y_{n-3}) & C(y_{n-2})
\end{array}
$$

$$
\begin{array}{cc}
\gamma & \kappa \\
-9\beta + \frac{9}{4}\alpha + \frac{9}{4}\varrho - \frac{9}{16}\kappa + \frac{9}{4}\sigma - \frac{9}{2} & \frac{3}{8}\varrho + 3\beta - \frac{3}{4}\alpha + \frac{3}{32}\gamma + \frac{15}{32}\kappa - \frac{3}{8}\sigma + \frac{3}{4} \\
\sigma & \varrho \\
3\beta - \frac{3}{4}\alpha - \frac{3}{4}\varrho + \frac{1}{16}\gamma + \frac{3}{16}\kappa & -\beta + \frac{1}{4}\alpha + \frac{5}{8}\varrho - \frac{1}{32}\gamma - \frac{3}{32}\kappa + \frac{1}{8}\sigma + \frac{3}{4} \\
\hline
C(y_{n-1}) & C(y_n)
\end{array},
$$

defining the fourth order method for $n \geqslant 3$.

A similar procedure can be used to design BDF-CF methods of order up to 6. It is not yet clear if one can obtain stable methods of order higher than 6 in this manner, since the classical k-step BDF methods are only stable up to to $k \leqslant 6$.

3 Some Convergence Results for the BDF-CF methods

We shall follow the strategy used by Hairer *et al.* [10, 9] to justify the convergence of the BDF-CF methods (2.1) when applied to the DAE (1.1). We begin with an existence and uniqueness theorem similar to the one in [10, Thm3.1,p.482].

Theorem 3.1. *Suppose that the initial values $y_j,\ z_j,\ \ j = 0, \dots, k-1$, satisfy*

$$
y_j - y(t_j) = \mathcal{O}(h), \quad z_j - z(t_j) = \mathcal{O}(h), \quad g(y_j) = \mathcal{O}(h^2). \tag{3.1}
$$

Then the nonlinear system

$$
\begin{aligned}
\alpha_k y_k + \sum_{i=0}^{k-1} \alpha_i \varphi_i y_i \quad &= \quad hf(y_k, z_k), &(3.2\text{a}) \\
0 \quad &= \quad g(y_k) &(3.2\text{b})
\end{aligned}
$$

as in (1.3) with $\alpha_k \neq 0$, has a solution for $h \leqslant h_0$. Furthermore, this solution is unique and satisfies

$$
y_k - y(t_k) = \mathcal{O}(h), \quad z_k - z(t_k) = \mathcal{O}(h). \tag{3.3}
$$

The proof follows the pattern used by Hairer and Wanner [10, Thm3.1, p.482] with minor modifications.

Proof. We set

$$
\eta = -\sum_{i=0}^{k-1} \frac{\alpha_i}{\alpha_k} \varphi_i y_i, \tag{3.4}
$$

and define ζ close to $z(t_k)$ such that

$$
g_y(\eta)\big(f(\eta, \zeta) + C(\eta)\eta\big) = \mathcal{O}(h). \tag{3.5}
$$

We then replace h/α_k by a new step size which we again denote by h, without loss of generality. The system (3.2) becomes equivalent to

$$
\begin{aligned}
y_k \quad &= \quad \eta + hf(y_k, z_k), &(3.6\text{a}) \\
0 \quad &= \quad g(y_k), &(3.6\text{b})
\end{aligned}
$$

which is the backward Euler method with initial data (η, ζ). Thus we can apply "Theorem 3.1" of [9, p.31] to conclude the proof. It only suffices therefore to show that

$$\eta - y(t_k) = O(h), \quad \zeta - z(t_k) = O(h), \quad g(\eta) = O(h^2). \tag{3.7}$$

(a) The first part of (3.7) follows by using that $\varphi_i y_i = y_i + O(h)$ and $\sum_{i=0}^{k} \alpha_i = 0$, together with the assumptions in (3.1). Thus we get

$$\begin{aligned}\eta - y(t_k) &= -\frac{1}{\alpha_k}\sum_{i=0}^{k-1}\alpha_i(\varphi_i y_i - y(t_k)) \\ &= -\frac{1}{\alpha_k}\sum_{i=0}^{k-1}\alpha_i(y_i - y(t_k)) + O(h) \\ &= -\frac{1}{\alpha_k}\sum_{i=0}^{k-1}\alpha_i[(y_i - y(t_i)) + (y(t_i) - y(t_k))] + O(h).\end{aligned}$$

So that

$$\eta - y(t_k) = O(h).$$

(b) Lastly, using the constraint (1.2) and the fact that $g_y f_z$ is invertible, we see (via Taylor expansion) that

$$g_y(\eta)(f(\eta,\zeta) + C(\eta)\eta) = g_y(y(t_k))\, f_z(y(t_k), z(t_k)) \cdot (\zeta - z(t_k)) + O(\|\eta - y(t_k)\|) + O(h^2). \tag{3.8}$$

Inserting (3.5) we get

$$\zeta - z(t_k) = O(h).$$

(c) The proof of the third part of (3.7) follows exactly as in [10, Thm3.1,p.482].

□

The next theorem, which is proved exactly as in [10, Thm3.2, p.484], considers the influence of perturbations in the application of BDF-CF methods to (1.1).

Theorem 3.2. *Suppose y_k, z_k are given by (3.2) and consider perturbed values $\hat{y}_k, \hat{z}_k$ satisfying*

$$\alpha_k \hat{y}_k + \sum_{i=0}^{k-1}\alpha_i \hat{\varphi}_i \hat{y}_i = h f(\hat{y}_k, \hat{z}_k) + h\delta, \tag{3.9a}$$

$$0 = g(\hat{y}_k) + \theta \tag{3.9b}$$

where $\hat{\varphi}_i := \exp\left(\sum_{j=0}^{k-1} a_{i+1,j+1} hC(\hat{y}_j)\right), \quad i = 0, \ldots, k-1$. *In addition to the assumptions of Theorem 3.1, suppose that for* $j = 0, \ldots, k-1$,

$$\hat{y}_j - y_j = O(h), \quad \hat{z}_j - z_j = O(h), \quad \delta = O(h), \quad \theta = O(h^2). \tag{3.10}$$

Then, for $h \leqslant h_0$, we have the estimates

$$\|\hat{y}_k - y_k\| \leqslant Const\left(\|\Psi(\hat{Y}_0 - Y_0)\| + h\|\delta\| + \|\theta\|\right), \tag{3.11a}$$

$$\|\hat{z}_k - z_k\| \leqslant \frac{Const}{h}\left(\sum_{j=0}^{k-1}\|g_y(\hat{y}_k)(\hat{\varphi}_j\hat{y}_j - \varphi_j y_j)\| + h\|\Psi(\hat{Y}_0 - Y_0)\| + h\|\delta\| + \|\theta\|\right) \tag{3.11b}$$

where $\Psi(\hat{Y}_0 - Y_0) := (\hat{\varphi}_{k-1}\hat{y}_{k-1} - \varphi_{k-1}y_{k-1}, \ldots, \hat{\varphi}_0\hat{y}_0 - \varphi_0 y_0)^T$ *and* $\|\Psi(\hat{Y}_0 - Y_0)\| := \max_{0 \leqslant j \leqslant k-1}\|\hat{\varphi}_j\hat{y}_j - \varphi_j y_j\|$.

3.1 Local error

Suppose we consider exact initial values $y_j = y(t_j),\ z_j = z(t_j),\ j = 0, \ldots, k-1$, in the BDF-CF formula (3.2) and also choose in (3.9) $\hat{y}_j = y(t_j),\ \hat{z}_j = z(t_j),\ j = 0, \ldots, k$. Then we will have from (3.9) that $\theta = 0$, and by the construction of the BDF-CF methods the truncation error gives $\delta = O(h^p)$. Also, since we now have $y_j = \hat{y}_j,\ z_j = \hat{z}_j$ for $j < k$, we get the following local error estimate, as a consequence of the estimates of Theorem 3.2.

Theorem 3.3. *Suppose that the BDF-CF method (3.2) applied to the DAE (1.1) has a truncation error of order p (in the sense implied by (2.3)). Then its local error satisfies*

$$y_k - y(t_k) = O(h^{p+1}), \quad z_k - z(t_k) = O(h^p). \tag{3.12}$$

3.2 Global Error

We observe that the convergence of the BDF-CF methods will require that the matrix-valued function $C(y)$ is sufficiently smooth on the space spanned by the initial data at each advancement in time.

Remark 3.4. We have the following remarks on the global convergence of the methods.

(a) The result in Theorem 3.3 is still obtainable if we replace the terms $\|\Psi(\hat{Y}_0 - Y_0)\|$ and $\|g_y(\hat{y}_k)(\hat{\varphi}_j\hat{y}_j - \varphi_j y_j)\|$, $j = 0, \ldots, k-1$, in (3.11) by the approximation (linearization)

$$\|g_y(\hat{y}_k)(\hat{\varphi}_j\hat{y}_j - \varphi_j y_j)\| \leqslant \|g_y(\hat{y}_k)(\hat{y}_j - y_j)\| + O(h\|g_y(\hat{y}_k)\hat{y}_j - y_j\|), \tag{3.13a}$$
$$\|\Psi(\hat{Y}_0 - Y_0)\| \leqslant \|\Delta Y_0\| + O(h\|\Delta Y_0\|) \tag{3.13b}$$

where $\Delta Y_0 := (\hat{y}_{k-1} - y_{k-1}, \ldots, \hat{y}_0 - y_0)^T$ and $\|\Delta Y_0\| := \max\limits_{0\leqslant j\leqslant k-1} \|\hat{y}_j - y_j\|$. Such approximations are possible by using Taylor expansion methods, which in turn depend on the smoothness of the function $C(y)$.

(b) Using (3.13) appropriately we can follow the same proof as "Theorem 3.5" of [10, p.486] to obtain the convergence of the BDF-CF applied to the index 2 DAE (1.1). Thus according to "Theorem 3.5" of [10, p.486] we expect to get convergence of order $p = k$, for $k \leqslant 6$, in both the algebraic and differential variables, upon applying the $k-$step BDF-CF method as detailed out in Algorithm 1 on page 4. This is investigated numerically in the following two subsections.

3.3 Numerical example

We here consider the index 2 problem (see [11])

$$\begin{aligned} \dot{y}_1 &= y_1^2 + z + \cos t - 1, \\ \dot{y}_2 &= y_1^2 + y_2^2 - \sin t - 1, \quad t \in [1, 2], \\ 0 &= y_1^2 + y_2^2 - 1, \end{aligned} \tag{3.14}$$

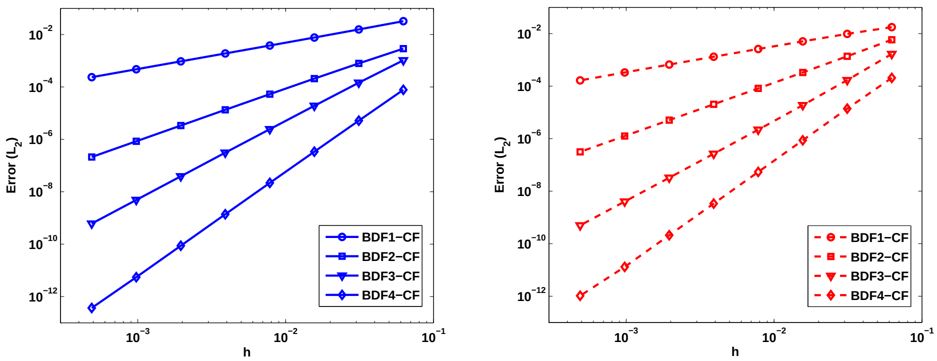
whose exact solution is given by

$$y_1(t) = \sin t, \quad y_2(t) = \cos t, \quad z(t) = \cos^2 t.$$

This DAE is comparable to (1.1) with

$$y = (y_1, y_2)^T, \quad g(y) = y_1^2 + y_2^2 - 1, \quad C(y) = \begin{pmatrix} y_1 & 0 \\ y_1 & y_2 \end{pmatrix}, \quad f = f(t, y, z) = \begin{pmatrix} z + \cos t - 1 \\ -\sin t - 1 \end{pmatrix}.$$

We now solve (3.14) using each of the methods BDF1-CF, BDF2-CF ($\gamma = 0$), BDF3-CF ($\alpha = \beta = \gamma = 0$) and BDF4-CF ($\alpha = \beta = \gamma = \sigma = \varrho = \kappa = 0$). Since the DAE system is small, we have computed the matrix exponentials using MATLAB's built in `expm` function. The global error (in the discrete L_2-norm, see Appendix A.1) at time $T = 2$, is plotted as a function of time step h, taking $h = 1/2^r$, $r = 4, \dots, 11$. As shown in Figure 1, we observe that for $k = 1, \dots, 4$, the method BDFk-CF gives convergence of order $p = k$ in both the differential and algebraic variables y and z. This agrees with the conclusion in Remark 3.4 for $k \leqslant 4$.



(a) Error in y (b) Error in z

Figure 1: Order of different BDF-CF methods to index 2 DAE (3.14). Errors are measured (in the discrete L_2-norm) at time $T = 2$ as functions of time step $h = 1/2^r$, $r = 4, \dots, 11$. (a) shows the errors in the differential variable y, while (b) shows the errors in the algebraic variable z.

3.4 Numerical test on Navier-Stokes

Next we consider the incompressible Navier-Stokes equations in $\mathbb{R}^2$,

$$\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla \bar{p} + \frac{1}{Re}\nabla^2 \mathbf{u}, \quad \text{in } \Omega, \tag{3.15a}$$

$$\nabla \cdot \mathbf{u} = 0, \quad \text{in } \Omega, \tag{3.15b}$$

with prescribed initial data and velocity boundary conditions. The constant Re is the Reynolds number, $\mathbf{x} = (x_1, x_2)^T \in \Omega \subset \mathbb{R}^2$, $t \in [0, T]$, while $\mathbf{u} = \mathbf{u}(\mathbf{x}, t) = (u_1, u_2)^T \in \mathbb{R}^2$ is the fluid velocity and $\bar{p} = \bar{p}(\mathbf{x}, t) \in \mathbb{R}$ is the pressure.

For the spatial discretization we employ a spectral element method (SEM) based on a standard Galerkin weak formulation. The approximation is done in $\mathbb{P}_N - \mathbb{P}_{N-2}$ compatible velocity-pressure discrete spaces, i.e., keeping the time variable t fixed, we approximate the velocity by a N-degree Lagrange polynomial based on Gauss-Lobatto-Legendre (GLL) nodes in each spatial coordinate, and the pressure by $(N-2)$-degree Lagrange polynomial based on Gauss-Legendre (GL) nodes. A more vivid description of this type of spatial discretization of Navier-Stokes is given by Fischer et.al [8]. The result is a semi-discrete (time-dependent) system of equations

$$B\dot{y} + C(y)y + Ay - D^T z = 0, \tag{3.16a}$$

$$Dy = 0 \tag{3.16b}$$

where $y = y(t) \in \mathbb{R}^n$, $z = z(t) \in \mathbb{R}^m$, represent the discrete velocity and pressure respectively, while the matrices A, B, C, D, D^T represent the discrete Poisson (negative Laplace), mass, convection, divergence and gradient operators respectively. The system (3.16) satisfies the requirements of the index 2 DAE (1.1), with $f(y,z) = B^{-1}(Ay - D^T z)$, $g(y) = Dy$, linear in their arguments. The matrix $g_y f_z = DB^{-1}D^T$ is invertible since B is positive definite. In fact, given $w \in \mathbb{R}^m$, $w \neq 0$, we have that

$$w^T(g_y f_z)w = (D^T w)^T B^{-1} D^T w > 0,$$

making $DB^{-1}D^T$ positive definite (assuming that the compatibility of the discrete spaces makes D to be of full rank). Thus the BDF-CF methods are applicable for the time integration of (3.16).

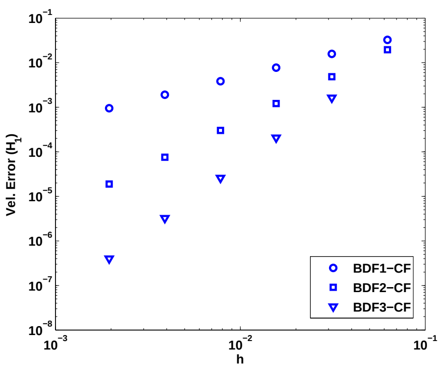
As a test example we consider the Taylor vortex problem [22, 26], with exact (analytic) solution given by

$$u_1 = -\cos(\pi x_1)\sin(\pi x_2)\exp(-2\pi^2 t/Re), \tag{3.17a}$$

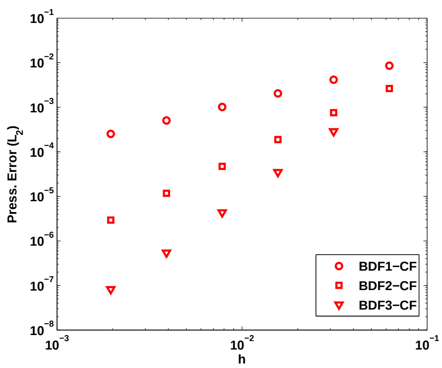
$$u_2 = \sin(\pi x_1)\cos(\pi x_2)\exp(-2\pi^2 t/Re), \tag{3.17b}$$

$$\bar{p} = -\frac{1}{4}[\cos(2\pi x_1) + \cos(2\pi x_2)]\exp(-4\pi^2 t/Re). \tag{3.17c}$$

In this example we have used Dirichlet boundary conditions on the spatial domain $\Omega = [-1,1]^2$, spectral element discretization (SEM) of order $N = 12$ with $Ne = 4$ rectangular elements, and the time integration is done up to time $T = 1$ using different constant stepsizes $h = T/2^r$, $r = 4,\ldots,9$. The error in both time and space is measured. The error (at time T) in the velocity is measured in the H_1-norm and the error in the pressure is measured in the L_2-norm (see Appendix A.1 for description of these norms). Figure 2 shows the temporal orders of convergence obtained with the methods BDF1-CF, BDF2-CF (with $\gamma = 0$) and BDF3-CF (with $\alpha = \beta = \gamma = 0$) applied to the semi-discrete incompressible Navier-Stokes problem (3.16). The Reynolds number used is $Re = 2\pi^2$. The same example was also used to test the fourth order method, BDF4-CF (not included in the figures), which showed a better overall convergence than the lower order methods. In this case, however, the temporal error is no longer dominant over the spatial error, and the overall error (both in time and space) is no longer monotonic with respect to h.



(a) Velocity



(b) Pressure

Figure 2: Temporal order test of different BDF-CF methods for the incompressible Navier-Stokes ($Re = 2\pi^2$). Taylor vortex problem on $x, y \in [-1,1]$, considered. We use Dirichlet BCs on $\Omega = [-1,1]^2$ and SEM of order $N = 12$ with $Ne = 4$ uniform rectangular elements. Errors are measured at time $T = 1$ and plotted as functions of time step $h = T/2^r$, $r = 4,\ldots,9$. (a) The errors in the velocity measured in the H_1-norm. (b) The errors in the pressure measured in the L_2-norm.

4 Stability of the BDF-CF methods

We study the stability of the BDF-CF methods, and make some comparisons with the IMEX multistep semi-explicit BDF (SBDF) methods of Ascher *et.al* [4], also studied in [18, 13]. The following remark shows a relation between the BDF-CF methods and the SBDF methods.

Remark 4.1. If we introduce linearizations of the form

$$\exp\left(hC(y_0)\right) y_1 \approx y_1 + hC(y_0)y_1$$

in the BDF-CF1, BDF-CF2 (with $\gamma = 0$) and BDF-CF3 (with $\alpha = 0$, $\beta = 2$, $\gamma = 1$), we obtain exactly the SBDF methods of Ascher *et.al* [4].

4.1 A nonlinear problem

The authors in [4] demonstrated the strong stability and time-step restrictions of the SBDF methods among others, in the treatment of convection-diffusion problems with small viscosity coefficients. An interesting observation is the improved stability of the BDF-CF over the SBDF methods at smaller viscosities. We consider the Burgers equation in $1D$

$$u_t + uu_x = \nu u_{xx}, \quad x \in (-1, 1), t > 0 \tag{4.1}$$

with initial condition $u(0, x) = \sin \pi x$, and homogeneous Dirichlet boundary conditions. We discretize in space via the Gauss-Lobatto-Chebyshev spectral collocation method to obtain an ODE of the form (2.2). This same test problem was considered in [4]. In Figure 3 we show the relative error in L_∞ grid-norm measured at time $T = 2$ for a range a viscosity parameters in the range $0.001 \leqslant \nu \leqslant 0.1$. For each time step $h = 1/10, 1/20,\ 1/40,\ 1/80$, we have used $N = 40$ spatial nodes. The reference or "exact" solution is computed for $N = 80$ spatial nodes using MATLAB's `ode45` built in function, with sufficiently small relative and absolute error tolerances.

An observation from Figure 3 seems to reveal that the BDF-CF methods are numerical more stable (with larger time step restrictions) than the SBDF methods. Unlike the BDF-CF methods, the SBDF methods give unbounded solutions at smaller viscosity parameters, especially as the Courant number increases with increasing time step h. The better performance of the BDF-CF methods at low viscosities is believed to be partly due to exponential integration of the convection term and partly due to the semi-Lagrangian computation of exponential flows (see also [7]).

4.2 Linear Stability

We now consider a linear stability analysis like the one done in [4], whereby we apply the methods to a simple problem of the type

$$\dot{y} = (\lambda + \hat{\imath}\upsilon)y, \tag{4.2}$$

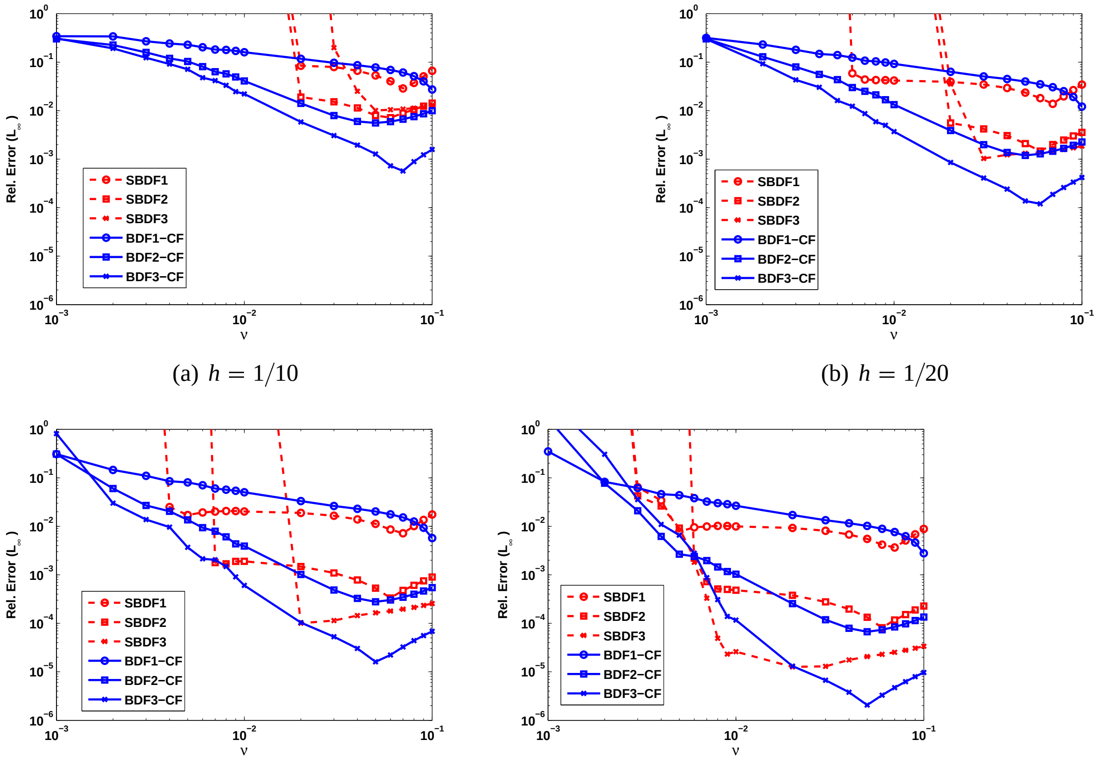
where $\lambda, \upsilon \in \mathbb{R}$, and $\hat{\imath}$ is the unit imaginary number satisfying $\hat{\imath}^2 = -1$. Notice that (4.2) is equivalent to (2.2) with $C(y) = \hat{\imath}\upsilon I$ and $f(y) = \lambda y$.

Let $\omega := (\lambda + \hat{\imath}\upsilon)h \in \mathbb{C}$, and let ω_R and ω_I denote the real and imaginary parts of ω respectively, suppressing the dependence on h. Applying the SBDF2 method to (4.2) yields the characteristic polynomial

$$\Phi(\tau; \omega) := (3 - 2\omega_R)\tau^2 - 4(1 + \hat{\imath}\omega_I)\tau + 2\hat{\imath}\omega_I + 1;$$

meanwhile the BDF2-CF method has characteristic polynomial

$$\Phi(\tau; \omega) := (3 - 2\omega_R)\tau^2 - 4e^{\hat{\imath}\omega_I}\tau + e^{2\hat{\imath}\omega_I}.$$



(a) $h = 1/10$ (b) $h = 1/20$

(c) $h = 1/40$ (d) $h = 1/80$

Figure 3: Burgers equation over a range of viscosity parameters. We use Dirichlet BCs on the domain $[-1, 1]$; $N = 40$. Relative errors (in the L_∞-norm) are measured at time $T = 2$ as functions of viscosity $\nu \in \{0.001, 0.002, \ldots, 0.01, 0.02, \ldots, 0.1\}$, for time steps $h = 1/10, 1/20, 1/40, 1/80$. SBDF1 and BDF1-CF are the first order methods. For BDF2-CF we used $\gamma = -1$, while for BDF3-CF we used $\alpha = 1, \beta = -13/2, \gamma = 3$. **Note:** The plot labels in (a) apply to all four diagrams.

The stability region is then given by the set

$$\mathcal{S} := \{\omega \in \mathbb{C} : |\max\{\tau : \Phi(\tau; \omega) = 0\}| \leqslant 1\}$$

In Table 1 we write down the characteristic polynomials of the second to fourth order BDF-CF and SBDF methods. Figure 4 shows the stability regions (shaded by contour lines) for these SBDF and BDF-CF methods.

We observe from Figure 4 that all the BDF-CF methods are A-stable. In particular the BDF2-CF has characteristic roots given by

$$\tau_{1,2} = e^{\hat{\imath}\omega_I}[2 \pm \sqrt{1 + 2\omega_R}]/(3 - 2\omega_R),$$

and it is easy to show that for $\omega_R \leqslant 0$ we have $|2 \pm \sqrt{1 + 2\omega_R}| \leqslant |3 - 2\omega_R|$, which implies that $|\tau_{1,2}| \leqslant 1$. In fact, given $\omega_R = -r,\ r \geqslant 0$,

$$|2 \pm \sqrt{1 + 2\omega_R}| = |2 \pm \sqrt{1 - 2r}| \leqslant 2 + \sqrt{|1 - 2r|}.$$

For $0 \leqslant r \leqslant 1/2$,

$$2 + \sqrt{|1 - 2r|} = 2 + \sqrt{1 - 2r} \leqslant 3 \leqslant 3 + 2r = |3 - 2\omega_R|;$$

Table 1: Characteristic polynomials for BDF-CF and SBDF methods

order	BDF-CF
2	$\left(\frac{3}{2}-\omega_R\right)\tau^2 - 2e^{\hat{\imath}\omega_I}\tau + \frac{1}{2}e^{2\hat{\imath}\omega_I}$
3	$\left(\frac{11}{6}-\omega_R\right)\tau^3 - 3e^{\hat{\imath}\omega_I}\tau^2 + \frac{3}{2}e^{2\hat{\imath}\omega_I}\tau - \frac{1}{3}e^{3\hat{\imath}\omega_I}$
4	$\left(\frac{25}{11}-\omega_R\right)\tau^4 - 4e^{\hat{\imath}\omega_I}\tau^3 + 3e^{2\hat{\imath}\omega_I}\tau^2 - \frac{4}{3}e^{3\hat{\imath}\omega_I} + \frac{1}{4}e^{4\hat{\imath}\omega_I}$
order	SBDF
2	$\left(\frac{3}{2}-\omega_R\right)\tau^2 - 2(1+\hat{\imath}\omega_I)\tau + \frac{1}{2}(1+2\hat{\imath}\omega_I)$
3	$\left(\frac{11}{6}-\omega_R\right)\tau^3 - 3(1+\hat{\imath}\omega_I)\tau^2 + \frac{3}{2}(1+2\hat{\imath}\omega_I)\tau - \frac{1}{3}(1+3\hat{\imath}\omega_I)$
4	$\left(\frac{25}{11}-\omega_R\right)\tau^4 - 4(1+\hat{\imath}\omega_I)\tau^3 + 3(1+2\hat{\imath}\omega_I)\tau^2 - \frac{4}{3}(1+3\hat{\imath}\omega_I) + \frac{1}{4}(1+4\hat{\imath}\omega_I)$

and for $r > 1/2$,

$$2 + \sqrt{|1-2r|} = 2 + \sqrt{2r-1} \leqslant 2 + 2r \leqslant 3 + 2r = |3 - 2\omega_R|.$$

On the other hand, the SBDF methods are only $A(\alpha)$-stable, in sense of [10, Definition2.1,p.250], with $\alpha < 90^\circ$ (see Figure 4). The SBDF4 shows even smaller stability region than the methods of lower order in its class.

We can thus conclude that for a linear convection-diffusion problem with constant coefficients and diffusion parameter $\nu > 0$, the time-step restrictions due to stability are much more relaxed in the BDF-CF methods than for the SBDF, both in the cases of small and large ν. The SBDF methods poses even more severe time-step restrictions for small ν. This is evident from the stability regions plotted in Figure 4.

Conclusion

So far we have derived new exponential multistep methods based on the BDF scheme, that can be applied to both ODEs and a class of index 2 DAEs in a semi-explicit or IMEX manner. The methods are shown to be unconditionally stable (e.g. for linear problems). Numerical experiments given reveal that when the methods are suitable for convection dominated convection diffusion problems when implemented in a semi-Lagrangian fashion. The convergence of the methods have been verified numerically on a Navier-Stokes problem. An interesting future work will be to analize or investigate the Courant-Friedrichs-Lewy (CFL) condition in the limiting case as the viscous term vanishes.

Acknowledgements

Our appreciations to professor Einar Rønquist (Mathematics department, NTNU, Norway) for his invaluable insights on the use spectral elements methods in the discretization of Navier Stokes equations. Further appreciations goes to post-doc student Tormod Bjøntegaard (Mathematics department, NTNU, Norway) for fruitful discussions on the implementation issues. Sincere thanks also go to the members of the numerical analysis group at NTNU for their treasured feedbacks during a seminar talk given on this topic in February 2010.

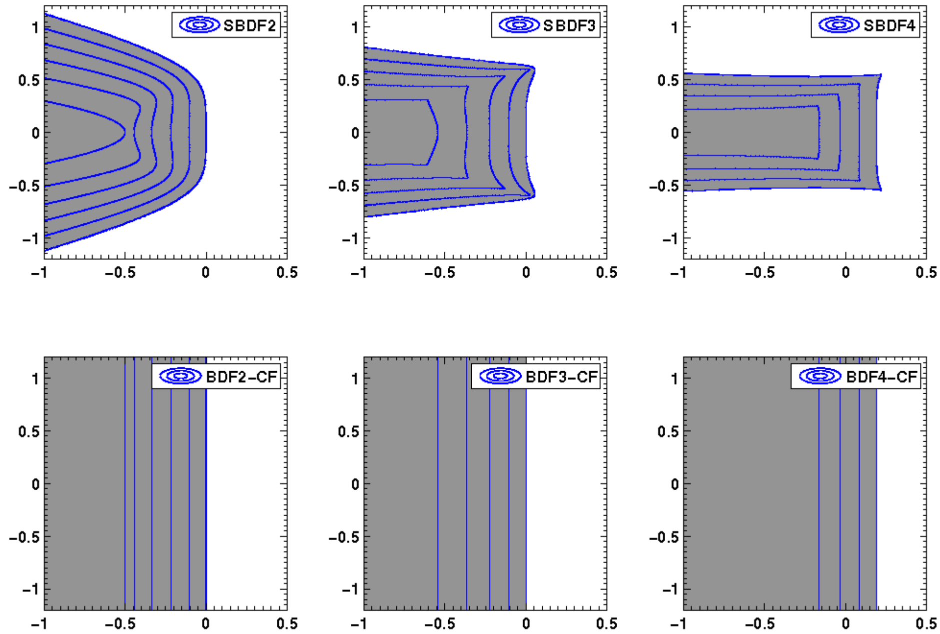


Figure 4: Stability domains $\mathcal{S} \subset \mathbb{C}$ (shaded gray, with contour lines) for SBDF and BDF-CF methods. Each domain $\mathcal{S}$ (partly shown) is unbounded and includes the whole negative real axis, and part/whole of the imaginary axis.

Appendix

A.1 Definition of norms

For a square-integrable function $\mathbf{u} : \Omega \to \mathbb{R}^n$, where $\Omega \subset \mathbf{R}^m$ is bounded and connected, the L_2- and H_1-norms, denoted $\|\cdot\|_{L_2}$, $\|\cdot\|_{H_1}$, are defined by

$$\|\mathbf{u}\|_{L_2}^2 := \sum_{i=1}^{n} \int_{\Omega} u_i^2 d\Omega, \tag{A.3}$$

and the H_1-norm is defined by

$$\|\mathbf{u}\|_{H_1}^2 := \sum_{i=1}^{n} \int_{\Omega} u_i^2 d\Omega. \tag{A.4}$$

In the spectral element approximations the continuous integrals of numerical solutions are accurately computed using Gauss quadrature rules.

Given a vector $y = (y_1, \ldots, y_K)^T \in \mathbb{R}^K$, the *discrete* L_2-norm, denoted $\|\cdot\|_2$, is defined by

$$\|y\|_2^2 := \sum_{j=1}^{K} y_j^2. \tag{A.5}$$

A.2 Order conditions for order 3 method BDF3-CF

$$3(a_{31}+a_{32}+a_{33})-\frac{3}{2}(a_{21}+a_{22}+a_{23})+\frac{1}{3}(a_{11}+a_{12}+a_{13})=1, \tag{A.6a}$$
$$3(a_{31}+a_{32}+a_{33})-\frac{1}{3}(a_{11}+a_{12}+a_{13})=2, \tag{A.6b}$$
$$3(a_{33}-a_{31})-\frac{3}{2}(a_{23}-a_{21})+\frac{1}{3}(a_{13}-a_{11})=2, \tag{A.6c}$$
$$3(a_{31}+a_{32}+a_{33})+\frac{1}{3}(a_{11}+a_{12}+a_{13})=4, \tag{A.6d}$$
$$3(a_{31}+a_{33})-\frac{3}{2}(a_{21}+a_{23})+\frac{1}{3}(a_{11}+a_{13})=4, \tag{A.6e}$$
$$3(a_{33}-a_{31})-\frac{1}{3}(a_{13}-a_{11})=4, \tag{A.6f}$$
$$3(a_{31}+a_{32}+a_{33})^2-\frac{3}{2}(a_{21}+a_{22}+a_{23})^2+\frac{1}{3}(a_{11}+a_{12}+a_{13})^2=0, \tag{A.6g}$$
$$3(a_{31}+a_{32}+a_{33})^2-\frac{1}{3}(a_{11}+a_{12}+a_{13})^2=0, \tag{A.6h}$$
$$3(a_{31}+a_{32}+a_{33})^3-\frac{3}{2}(a_{21}+a_{22}+a_{23})^3+\frac{1}{3}(a_{11}+a_{12}+a_{13})^3=0, \tag{A.6i}$$
$$\begin{aligned}3(a_{31}+a_{32}+a_{33})(a_{33}-a_{31})-\frac{3}{2}(a_{21}+a_{22}+a_{23})(a_{23}-a_{21})&\\+\frac{1}{3}(a_{11}+a_{12}+a_{13})(a_{13}-a_{11})=0.&\end{aligned} \tag{A.6j}$$

A.3 DIRK-CF methods

Suppose the pair $\{a_{ij}, b_i, c_i\}$ and $\{\tilde{a}_{ij}, \tilde{b}_i, \tilde{c}_i\}$, for $i, j = 1, \ldots, s$, define the coefficients of a s-stage additive partitioned RK method (for DIRK-CF the partitioned RK coefficients are such that the first is DIRK and the second is ERK). We define coefficients α_{il}^j, $\beta_l^j, l = 1, \ldots, J$, for some integer $J \geqslant 1$, such that

$$\tilde{a}_{ij} = \sum_{l=0}^{J} \alpha_{il}^j, \quad \tilde{b}_j = \sum_{l=0}^{J} \beta_l^j. \tag{A.7}$$

Then a direct application of the DIRK-CF methods to (1.1) for one time step $[t_n, t_n + h]$ is given by the following algorithm:

Algorithm 2. *DIRK-CF method*

---

for $i = 1$ ***to*** s ***do***

$$\begin{aligned}\varphi_i &= \exp\left(h\sum_k \alpha_{iJ}^k C(Y_k)\right)\cdot\ldots\cdot\exp\left(h\sum_k \alpha_{i1}^k C(Y_k)\right),\\ Y_i &= \varphi_i y_n + h\sum_j a_{ij}\varphi_i\varphi_j^{-1} f(Y_j, Z_j), &\text{(A.8a)}\\ 0 &= g(Y_i), &\text{(A.8b)}\end{aligned}$$

end for

$$
\begin{aligned}
\varphi_{s+1} &= \exp\left(h\sum_k \beta_J^k C(y_k)\right)\cdot \ldots \cdot \exp\left(h\sum_k \beta_1^k C(y_k)\right), \\
y_{n+1} &= \varphi_{s+1} y_n + h\sum_i b_i \varphi_i f(Y_i, Z_i), && \textbf{(}A.8c\textbf{)} \\
0 &= g(y_{n+1}), && \textbf{(}A.8d\textbf{)}
\end{aligned}
$$

---

which computes the numerical solution y_{n+1} from a given initial value y_n. The values Y_i, Z_i for $i = 1, \ldots, s$, denote the numerical approximations of the stage values $y(t_i), z(t_i)$ respectively, and $\sum_j$ denotes $\sum_{j=1}^{s}$. The method is easy to implement when the coefficients $\{a_{ij}, b_i, c_i\},\ i, j = 1, \ldots, s$, defines a DIRK method. Typically the constraints, $0 = g(Y_i),\ 0 = g(y_{n+1})$, are enforced via a projection technique [2, 10, 21, 22]. If the DIRK method is stiffly accurate we immediately obtain that $z_{n+1} = Z_s$, otherwise if the RK matrix (a_{ij}) is invertible, we get

$$
z_{n+1} = z_n + \sum_{ij=1}^{s} \omega_{ij}(Z_j - z_n), \tag{A.9}
$$

where ω_{ij} are entries of the inverse of the RK matrix (a_{ij}) (see [10]).

References

[1] R. Alexander, *Diagonally Implicit Runge-Kutta methods for stiff o.d.e.'s*, SIAM J. Numer. Anal. **14** (1977), no. 6, 1006–1021.

[2] U. M. Ascher and L. R. Petzold, *Projected implicit Runge-Kutta methods for differential-algebraic equations*, SIAM J. Numer. Anal. **28** (1991), no. 4, 1097–1120.

[3] U. M. Ascher, S. J. Ruuth, and R. J. Spiteri, *Implicit-explicit Runge-Kutta methods for time-dependent partial differential equations*, Appl. Numer. Math. **25** (1997), 151–167.

[4] U. M. Ascher, S. J. Ruuth, and B. T. R. Wetton, *Implicit-explicit methods for time-dependent partial differential equations*, SIAM J. Numer. Anal. **32** (1995), no. 3, 797–823.

[5] M. P. Calvo and C. Palencia, *A class of explicit multistep exponential integrators for semilinear problems*, Numer. Math. **102** (2006), no. 3, 367–381.

[6] E. Celledoni, *Eulerian and semi-Lagrangian commutator-free exponential integrators*, CRM Proceedings and Lecture Notes **39** (2005), 77–90.

[7] E. Celledoni and B. K. Kometa, *Semi-Lagrangian Runge-Kutta exponential integrators for convection dominated problems*, J. Sci. Comput. **41** (2009), no. 1, 139–164.

[8] P. F. Fischer, G. W. Kruse, and F. Loth, *Spectral element method for transitional flows in complex geometries*, J. Sc. Comput. **17** (2002), no. 1–4, 81–98.

[9] E. Hairer, Ch. Lubich, and M. Roche, *The numerical solution of differential-algebraic systems by Runge-Kutta methods*, Lecture Notes in Mathematics, vol. 1409, Springer-Verlag, Berlin, 1989.

[10] E. Hairer and G. Wanner, *Solving ordinary differential equations. II*, second ed., Springer Series in Computational Mathematics, vol. 14, Springer-Verlag, Berlin, 1996, Stiff and differential-algebraic problems.

[11] I. Higueras and T. Roldán, *Starting algorithms for a class of RK methods for index-2 DAEs*, Comput. Math. Appl. **49** (2005), no. 7-8, 1081–1099.

[12] S. Hugues and A. Randriamampianina, *An improved projection scheme applied to pseudospectral methods for the incompressible Navier-Stokes equations*, Internat. J. Numer. Methods Fluids **28** (1998), no. 3, 501–521.

[13] W. Hundsdorfer and S. J. Ruuth, *IMEX extensions of linear multistep methods with general monotonicity and boundedness properties*, J. Comput. Phys. **225** (2007), no. 2, 2016–2042.

[14] L. O. Jay, *Convergence of a class of Runge-Kutta methods for differential-algebraic systems of index 2*, BIT **33** (1993), no. 1, 137–150.

[15] ______, *Solution of index 2 implicit differential-algebraic equations by Lobatto Runge-Kutta methods*, BIT **43** (2003), no. 1, 93–106.

[16] ______, *Specialized Runge-Kutta methods for index 2 differential-algebraic equations*, Math. Comp. **75** (2006), no. 254, 641–654 (electronic).

[17] G. E. Karniadakis, M. Israeli, and S. A. Orszag, *High-order splitting methods for the incompressible Navier-Stokes equations*, J. Comput. Phys. **97** (1991), no. 2, 414–443.

[18] A. Kassam and L. N. Trefethen, *Fourth-order time-stepping for stiff PDEs*, SIAM J. Sci. Comput. **26** (2005), no. 4, 1214–1233 (electronic).

[19] C. A. Kennedy and M. H. Carpenter, *Additive Runge-Kutta schemes for convection-diffusion-reaction equations*, Appl. Numer. Math. **44** (2003), no. 1-2, 139–181.

[20] A. Kværnø, *Singly diagonally implicit Runge-Kutta methods with an explicit first stage*, BIT **44** (2004), no. 3, 489–502.

[21] Ch. Lubich, *On projected Runge-Kutta methods for differential-algebraic equations*, BIT **31** (1991), no. 3, 545–550.

[22] Y. Maday, A. T. Patera, and E. M. Rønquist, *An operator-integration-factor splitting method for time-dependent problems: application to incompressible fluid flow*, J. Sci. Comput. **5** (1990), no. 4, 263–292.

[23] A. Ostermann and M. Thalhammer, *Positivity of exponential multistep methods*, Numerical mathematics and advanced applications, Springer, Berlin, 2006, pp. 564–571.

[24] R. Peyret, *Spectral methods for incompressible vicous flow*, Appl. Math. Sc., vol. 148, Springer, Berlin, 2000.

[25] J. Rang, *Design of DIRK schemes for solving Navier-Stokes equations*, Informatikbericht 2007-02, Technische Universitat Braunschweig (2007), no. 2.

[26] K. Shahbazi, P. F. Fischer, and C. R. Ethier, *A high-order discontinuous Galerkin method for the unsteady incompressible Navier-Stokes equations*, J. Comput. Phys. **222** (2007), no. 1, 391–407.

[27] J. Wensch, O. Knoth, and A. Galant, *Multirate infinitesimal step methods for atmospheric flow simulation*, BIT **49** (2009), no. 2, 449–473.

[28] D. Xiu and G. E. Karniadakis, *A semi-Lagrangian high-order method for Navier-Stokes equations*, J. Comput. Phy. **172** (2001), 658–684.