SEMI-LAGRANGIAN MULTISTEP EXPONENTIAL INTEGRATORS FOR INDEX 2 DIFFERENTIAL ALGEBRAIC SYSTEMS

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joint work with
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Problem statement

We consider **index-2 differential-algebraic equations** (DAEs) of the form

\[
\begin{align*}
\dot{y} &= C(y)y + f(y, z), \\
0 &= g(y),
\end{align*}
\]

with consistent initial data \( y(0) = y_0, z(0) = z_0 \), where

- \( y = y(t) \in \mathbb{R}^n, \ z = z(t) \in \mathbb{R}^m \), for all \( t \in [0, T] \);
- \( f : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^n, \ g : \mathbb{R}^n \rightarrow \mathbb{R}^m \);
- \( C = C(y) : \mathbb{R}^n \rightarrow \mathbb{R}^{n \times n} \) is a matrix-valued function of \( y \).
- **Application:** Navier-Stokes, convection diffusion PDEs, convection dominated flows.
Keywords

— Exponential integrators
— Backward differentiation formula (BDF)
— Implicit-explicit (IMEX) time splitting scheme
— semi-Langrangian methods
PRESENTATION OF METHOD

Given $k$ initial values $y_0, \ldots, y_{k-1}$, we define the semi-explicit $k$-step exponential BDF method (named BDF-CF) as follows:
Find $(y_k, z_k)$ such that

$$
\alpha_k y_k + \sum_{i=0}^{k-1} \alpha_i \varphi_i y_i = hf(y_k, z_k),
$$

(3)

$$
0 = g(y_k)
$$

(4)

where

— $\varphi_i := \exp \left( \sum_{j=0}^{k-1} a_{i+1,j+1} hC(y_j) \right), i = 0, \ldots, k - 1,$
— $a_{ij} \in \mathbb{R}, i, j = 1, \ldots, k$, are coefficients of the method,
— $\alpha_i, i = 0, \ldots, k$, are coefficients of the linear $k$-step classical BDF method.
P R E S E N T A T I O N O F M E T H O D

Thus given a discrete time interval $0 = t_0, \ldots, t_K = T$ and initial data $y_0, \ldots, y_{k-1}, 1 \leq k \leq K$, we describe a $k$-step BDF-CF method as follows

**Algorithm**

**for** $n = k$ **to** $K$ **find** $(y_n, z_n)$ **such that**

\[
\forall i = 0, \ldots, k - 1, \varphi_{ni} = \exp \left( h \sum_{j=0}^{k-1} a_{i+1,j+1} C(y_{n-k+j}) \right), \quad (5)
\]

\[
\alpha_k y_n + \sum_{i=0}^{k-1} \alpha_i \varphi_{ni} y_{n-k+i} = hf(y_n, z_n), \quad (6)
\]

\[
0 = g(y_n) \quad (7)
\]

**end for**
**Presentation of method**

We can represent a $k$-step BDF-CF method in terms of its coefficients as in the following table

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

So that for each $n \geq k - 1$ the method solves for the unknown values, $y_{n+1}, z_{n+1}$, given the initial values $y_{n-k+1}, \ldots, y_n$. 
Derivation of method

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

Without loss of generality, we consider the ODE

$$\dot{y} = C(y)y + f(y). \quad (8)$$

Assume that the truncation error $\tau_2(h)$ for a two-step method is given by

$$\frac{1}{h} \left[ \frac{3}{2} \hat{y}_2 - 2\hat{\varphi}_1 \hat{y}_1 + \frac{1}{2} \hat{\varphi}_0 \hat{y}_0 \right] = f(\hat{y}_2) + \tau_2(h). \quad (9)$$

For a classical second order BDF method we have

$$\frac{1}{h} \left[ \frac{3}{2} \hat{y}_2 - 2\hat{y}_1 + \frac{1}{2} \hat{y}_0 \right] = C(\hat{y}_2)\hat{y}_2 + f(\hat{y}_2) + O(h^2). \quad (10)$$
Derivation of method

So if $\tau_2(h) = O(h^2)$, combining (9) and (10) will give

$$\frac{1}{h} \left[ 2 \hat{\varphi}_1 \hat{y}_1 - \frac{1}{2} \hat{\varphi}_0 \hat{y}_0 - 2 \hat{y}_1 + \frac{1}{2} \hat{y}_0 \right] - C(\hat{y}_2) \hat{y}_2 = O(h^2), \quad (11)$$

which is a reasonable requirement for a second order method.

Applying Taylor expansion on (11) and comparing coefficients of like differentials and powers of $h$ we obtain the following order conditions on the coefficients for order 2

$$2(a_{11} + a_{21}) - \frac{1}{2} (a_{12} + a_{22}) - 1 = 0,$$

$$-2a_{11} + \frac{1}{2} a_{12} - 1 = 0,$$

$$\frac{1}{2} (a_{21} + a_{22}) - 1 = 0,$$

$$(a_{11} + a_{21})^2 - \frac{1}{4} (a_{12} + a_{22})^2 = 0.$$
Derivation of method

Solving this system yields a one-parameter method, illustrated in the following table

<table>
<thead>
<tr>
<th></th>
<th>2(1 + 2γ)</th>
<th>−4γ</th>
</tr>
</thead>
<tbody>
<tr>
<td>y₀</td>
<td>γ</td>
<td>1 − γ</td>
</tr>
<tr>
<td>y₁</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(C(y₀)) (C(y₁))

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

\[
\frac{3}{2} y_2 - 2 \varphi_1 y_1 + \frac{1}{2} \varphi_0 y_0 = hf(y_2) \tag{12}
\]

where

\[
\varphi_0 = \exp \left(2(1 + \gamma)hc(y_0) - 4\gamma hc(y_1)\right),
\]

\[
\varphi_1 = \exp \left(\gamma hc(y_0) + (1 - \gamma)hc(y_1)\right).
\]

Applied to the DAE we get

\[
\frac{1}{h} \left[\frac{3}{2} y_2 - 2 \varphi_1 y_0 + \frac{1}{2} \varphi_0 y_0\right] = f(y_2, z_2),
\]

\[
0 = g(y_2). \tag{13}
\]
# Derivation of method

Higher order methods are derived in a similar manner!!

Coefficients for the third order method (**BDF3-CF**)

| $y_0$ | $\frac{33}{2} - \frac{9}{4}\beta - 9\gamma$ | $-18 + 9\alpha + \frac{9}{2}\beta + 9\gamma$ | $\frac{9}{2} - 9\alpha - \frac{9}{4}\beta$ |
| $y_1$ | $3 + 2\alpha - \frac{1}{2}\beta - 2\gamma$ | $\beta$ | $-1 - 2\alpha - \frac{1}{2}\beta + 2\gamma$ |
| $y_2$ | $\alpha$ | $1 - \alpha - \gamma$ | $\gamma$ |

with parameters $\alpha, \beta, \gamma \in \mathbb{R}$.
Derivation of method

Coefficients for the fourth order method (BDF4-CF)

\[
\begin{array}{cccccc}
  y_0 & a_{11} & a_{12} & \gamma & \kappa \\
  y_1 & a_{21} & a_{22} & a_{23} & a_{24} \\
  y_2 & \alpha & a_{32} & \sigma & \rho \\
  y_3 & \beta & a_{42} & a_{43} & a_{44} \\
\end{array}
\]

\[
\begin{array}{cccc}
  C(y_0) & C(y_1) & C(y_2) & C(y_3) \\
\end{array}
\]

with parameters \(\alpha, \beta, \gamma, \rho, \sigma, \kappa \in \mathbb{R}\).
Derivation of method

where

\[ a_{11} = 4\alpha - 4\sigma - 8\varphi + 12 + \gamma + 2\kappa, \]
\[ a_{12} = -4\alpha + 8\varphi - 2\gamma - 3\kappa - 8 + 4\sigma, \]
\[ a_{21} = -3\beta + 3\alpha - \frac{3}{2}\varphi + \frac{3}{16}\gamma + \frac{3}{8}\kappa - \frac{3}{4}\sigma + \frac{3}{2}, \]
\[ a_{22} = 9\beta - \frac{9}{2}\alpha - \frac{9}{8}\varphi - \frac{9}{32}\gamma - \frac{9}{32}\kappa - \frac{9}{8}\sigma + \frac{21}{4}, \]
\[ a_{32} = 2 - \varphi - \sigma - \alpha, \]
**Derivation of method**

where

\[
a_{42} = \frac{1}{4} - 3\beta + \frac{1}{2}\alpha + \frac{1}{8}\varphi - \frac{3}{32}\kappa - \frac{1}{32}\gamma - \frac{1}{8}\sigma,
\]

\[
a_{23} = -9\beta + \frac{9}{4}\alpha + \frac{9}{4}\varphi - \frac{9}{16}\kappa + \frac{9}{4}\sigma - \frac{9}{2},
\]

\[
a_{24} = \frac{3}{8}\varphi + 3\beta - \frac{3}{4}\alpha + \frac{3}{32}\gamma + \frac{15}{32}\kappa - \frac{3}{8}\sigma + \frac{3}{4},
\]

\[
a_{43} = 3\beta - \frac{3}{4}\alpha - \frac{3}{4}\varphi + \frac{1}{16}\gamma + \frac{3}{16}\kappa,
\]

\[
a_{44} = -\beta + \frac{1}{4}\alpha + \frac{5}{8}\varphi - \frac{1}{32}\gamma - \frac{3}{32}\kappa + \frac{1}{8}\sigma + \frac{3}{4}.
\]
**Linear stability**

We now consider a linear stability analysis like the one done in [Ascher et al., 1995]; [Hundsdorfer et al., 2007], whereby we apply the methods to a simple problem of the type

\[
\dot{y} = (\lambda + \hat{i} \upsilon)y,
\]

where \( \lambda, \upsilon \in \mathbb{R} \), and \( \hat{i} \) is the unit imaginary number satisfying \( \hat{i}^2 = -1 \).

— Let \( \omega := (\lambda + \hat{i} \upsilon)h \in \mathbb{C} \), and let \( \omega_R \) and \( \omega_I \) denote the real and imaginary parts of \( \omega \) respectively, suppressing the dependence on \( h \).

— Denote by \( \Phi(\tau; \omega) \) the characteristic polynomial (in \( \tau \)) of a given method applied to (14).

— Then the stability region for the method is defined by (see [Ascher et al., 1995])

\[
S := \{ \omega \in \mathbb{C} : | \max\{\tau : \Phi(\tau; \omega) = 0\}| \leq 1 \}
\]
# Linear Stability

The characteristic polynomials of the **SBDF** methods of [Ascher et al., 1995] and those of BDF-CF methods.

<table>
<thead>
<tr>
<th>order</th>
<th>BDF-CF</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$\left(\frac{3}{2} - \omega_R\right)\tau^2 - 2e^{i\omega_1\tau} + \frac{1}{2}e^{2i\omega_1\tau}$</td>
</tr>
<tr>
<td>3</td>
<td>$\left(\frac{11}{6} - \omega_R\right)\tau^3 - 3e^{i\omega_1\tau^2} + \frac{3}{2}e^{2i\omega_1\tau} - \frac{1}{3}e^{3i\omega_1\tau}$</td>
</tr>
<tr>
<td>4</td>
<td>$\left(\frac{25}{11} - \omega_R\right)\tau^4 - 4e^{i\omega_1\tau^3} + 3e^{2i\omega_1\tau^2} - \frac{4}{3}e^{3i\omega_1\tau} + \frac{1}{4}e^{4i\omega_1\tau}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>order</th>
<th>SBDF</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$\left(\frac{3}{2} - \omega_R\right)\tau^2 - 2(1 + \hat{i}\omega_1)\tau + \frac{1}{2}(1 + 2\hat{i}\omega_1)$</td>
</tr>
<tr>
<td>3</td>
<td>$\left(\frac{11}{6} - \omega_R\right)\tau^3 - 3(1 + \hat{i}\omega_1)\tau^2 + \frac{3}{2}(1 + 2\hat{i}\omega_1)\tau - \frac{1}{3}(1 + 3\hat{i}\omega_1)$</td>
</tr>
<tr>
<td>4</td>
<td>$\left(\frac{25}{11} - \omega_R\right)\tau^4 - 4(1 + \hat{i}\omega_1)\tau^3 + 3(1 + 2\hat{i}\omega_1)\tau^2 - \frac{4}{3}(1 + 3\hat{i}\omega_1) + \frac{1}{4}(1 + 4\hat{i}\omega_1)$</td>
</tr>
</tbody>
</table>
LINEAR STABILITY

Stability domains $S \subseteq \mathbb{C}$ (shaded) for SBDF and BDF-CF methods.
NONLINEAR TEST PROBLEM

We consider the Burgers equation in $1D$

\[ u_t + uu_x = \nu u_{xx}, \quad x \in (-1, 1), \ t > 0 \quad (15) \]

with initial condition $u(0, x) = \sin \pi x$, and homogeneous Dirichlet boundary conditions.
NONLINEAR TEST PROBLEM

— Spatial discretization: Gauss-Lobatto-Chebyshev spectral collocation method with \( N = 40 \) nodes.

— Test problem also considered by [Ascher et al., 1997].

— Relative error in \( L_\infty \) grid-norm is measured at time \( T = 2 \) as a function of viscosity, \( 0.001 \leq \nu \leq 0.1 \).

— The reference or “exact” solution is computed for \( N = 80 \) spatial nodes using MATLABs build-in \texttt{ode45} function.

— For each time steps \( h = 1/10, 1/20, 1/40, 1/80 \), compare the performance of SBDF and BDF-CF.

— Exponential flows in the BDF-CF methods are evaluated in a semi-Lagrangian fashion [Celledoni et al. 2009].
NONLINEAR TEST PROBLEM

Figure: $h = 1/80$
NONLINEAR TEST PROBLEM

Figure: $h = 1/40$
NONLINEAR TEST PROBLEM

Figure: $h = 1/20$

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NONLINEAR TEST PROBLEM

Figure: $h = 1/10$
**Nonlinear test problem- Observations**

1. Courant number increases with increasing time step.
2. BDF-CF methods perform better than SBDF methods at low viscosities.

Reason is two-fold (see also [Celledoni et al. 2009])

1. exponential integration of the convection term (stiff term at low viscosity)
2. semi-Lagrangian computation of exponential flows
On the Convergence Theory

The convergence of the BDF-CF methods applied to our class of DAE has been investigated following a sequence of steps used for the standard BDF methods by [Hairer et al. 1989,1996].

— Perturbation estimates.

— Local error estimates.

— Global error estimates.

— At each stage the essential modification to the proofs will be to linearize the exponential flow $\phi y = y + O(h)$.

So that a $k$-step BDF-CF method will provide a convergence of order $p = k, \ 1 \leq k \leq 6$, provided the initial values are accurate to order $O(h^{p+1})$. 

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A simple test case

We here consider the index 2 problem [Higuera et al. 2005]

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

(16)

whose exact solution is given by

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

Splitting as follows:

\[
\begin{align*}
\mathbf{C}(\mathbf{y}) &= \begin{bmatrix} y_1 & 0 \\ y_1 & y_2 \end{bmatrix}, \\
f(t, y, z) &= \begin{bmatrix} z + \cos t - 1 \\ -\sin t - 1 \end{bmatrix}, \\
g(y) &= y_1^2 + y_2^2 - 1.
\end{align*}
\]
A SIMPLE TEST CASE

— Methods: BDF1-CF, BDF2-CF ($\gamma = 0$), BDF3-CF ($\alpha = \beta = \gamma = 0$) and BDF4-CF ($\alpha = \beta = \gamma = \sigma = \varphi = \kappa = 0$).

— Compute the matrix exponentials using MATLAB’s built in expm function.

— Measure global error (in the discrete $L_2$-norm) at time $T = 2$.

— Error is plotted as a function of time step $h$, taking $h = 1/2^r$, $r = 4, \ldots, 11$. 
A SIMPLE TEST CASE

Error in $y$

Error in $z$
**Numerical test on Navier-Stokes**

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

\[
    u_t + (u \cdot \nabla) u = -\nabla \bar{p} + \frac{1}{Re} \nabla^2 u \quad \text{in} \quad \Omega \times (0, T],
\]

\[
    \nabla \cdot u = 0 \quad \text{in} \quad \Omega \times (0, T],
\]

with prescribed initial data and velocity boundary conditions.

$Re =$ Reynolds number,

$u = u(x, t) = [u_1, u_2]^T \in \mathbb{R}^2$ is the fluid velocity and

$\bar{p} = \bar{p}(x, t) \in \mathbb{R}$ is the pressure,

$x = (x_1, x_2) \in \Omega \subset \mathbb{R}^2, \ t \in [0, T]$.
**Numerical test on Navier-Stokes**

For the spatial discretization [Fischer et al. 2002]

- Spectral element method (SEM) based on a standard Galerkin weak formulation
- $P_N - P_{N-2}$ compatible velocity-pressure discrete spaces
- Gauss-Lobatto-Legendre (GLL) nodes for velocity
- Gauss-Legendre (GL) nodes for pressure
- Dirichlet boundary conditions on the spatial domain $\Omega = [-1, 1]^2$
**Numerical test on Navier-Stokes**

The result is a semi-discrete (time-dependent) system of equations (within the considered class of DAEs)

\[
B\dot{y} + C(y)y + Ay - D^Tz = 0, \quad (19)
\]

\[
Dy = 0 \quad (20)
\]

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.
Numerical test on Navier-Stokes

As a test example we consider the Taylor vortex problem [Maday et al., 1990, Shahbazi et al., 2007] with exact (PDE) solution given by

\[ u = \begin{bmatrix} -\cos(\pi x_1) \sin(\pi x_2) \\ \sin(\pi x_1) \cos(\pi x_2) \end{bmatrix} \exp(-2\pi^2 t/Re), \] \hspace{1cm} (21)

\[ \bar{p} = -\frac{1}{4} \left( \cos(2\pi x_1) + \cos(2\pi x_2) \right) \exp(-4\pi^2 t/Re), \] \hspace{1cm} (22)
**Numerical test on Navier-Stokes**

- Methods: BDF2-CF (with $\gamma = 0$), BDF3-CF (with $\alpha = \beta = \gamma = 0$) and BDF4-CF (with $\alpha = \kappa = -1, \beta = \gamma = 0, \sigma = 3, \varphi = 1/2$)
- semi-Lagrangian method for exponential flows
- spectral element discretization of order $N = 12$ with $Ne = 4$ rectangular element
- time integration is done upto time $T = 1$ using different constant time steps $h = T/2^k, k = 4, \ldots, 9$
- global error in the velocity is measured in the $H_1$-norm
- global error in the pressure is measured in the $L_2$-norm
- $Re = 2\pi^2$. 
**Numerical test on Navier-Stokes**

Velocity error ($H_1$-norm)  
Pressure error ($L_2$-norm)

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CONCLUSION

— We have constructed IMEX exponential integrators of upto order 4 based on the BDF.
— Verified the linear stability of the methods.
— Still need to investigate the potential of these methods for solving convection dominated problems or Navier-Stokes at high Reynolds number.
— Thanks for your attention!