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

$$\dot{y} = \mathbf{C}(y)y + f(y,z), \quad (1)$$
$$0 = g(y), \quad (2)$$

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

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KEYWORDS

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

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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

$$\alpha_k y_k + \sum_{i=0}^{k-1} \alpha_i \boldsymbol{\varphi}_i y_i = hf(y_k, z_k), \quad (3)$$

$$0 = g(y_k) \quad (4)$$

where

- $\boldsymbol{\varphi}_i := \exp\left(\sum_{j=0}^{k-1} a_{i+1,j+1} h\boldsymbol{C}(y_j)\right)$, $i = 0, \ldots, k-1$,
- $a_{ij} \in \mathbb{R}$, $i, j = 1, \ldots, k$, are coefficients of the method,
- α_i, $i = 0, \ldots, k$, are coefficients of the linear k-step classical BDF method.

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Presentation of method

Thus given a discrete time interval $0 = t_0, \ldots, t_K = T$ 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

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

$$\forall i = 0, \ldots, k-1,\ \boldsymbol{\varphi}_{ni} = \exp\left(h \sum_{j=0}^{k-1} a_{i+1,j+1} \mathbf{C}(y_{n-k+j})\right), \quad (5)$$

$$\alpha_k y_n + \sum_{i=0}^{k-1} \alpha_i \boldsymbol{\varphi}_{ni} y_{n-k+i} = hf(y_n, z_n), \quad (6)$$

$$0 = g(y_n) \quad (7)$$

end for

Presentation of method

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

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

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 $y_{n-k+1}, \dots, y_n$.

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Derivation of method

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

Without loss of generality, we consider the ODE

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

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

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

For a classical second order BDF method we have

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

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Derivation of method

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

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

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

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

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Derivation of method

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

y_0	$2(1+2\gamma)$	-4γ
y_1	γ	$1-\gamma$
	$\boldsymbol{C}(y_0)$	$\boldsymbol{C}(y_1)$

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

$$\frac{3}{2}y_2 - 2\boldsymbol{\varphi}_1 y_1 + \frac{1}{2}\boldsymbol{\varphi}_0 y_0 = hf(y_2) \tag{12}$$

where
$$\boldsymbol{\varphi}_0 = \exp\left(2(1+\gamma)h\boldsymbol{C}(y_0) - 4\gamma h\boldsymbol{C}(y_1)\right),$$
$$\boldsymbol{\varphi}_1 = \exp\left(\gamma h\boldsymbol{C}(y_0) + (1-\gamma)h\boldsymbol{C}(y_1)\right).$$

Applied to the **DAE** we get

$$\frac{1}{h}[\frac{3}{2}y_2 - 2\boldsymbol{\varphi}_1 y_0 + \frac{1}{2}\boldsymbol{\varphi}_0 y_0] = f(y_2, z_2),$$
$$0 = g(y_2). \tag{13}$$

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Derivation of method

Higher order methods are derived in a similar manner!!

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

$$
\begin{array}{c|ccc}
y_0 & \frac{33}{2} - \frac{9}{4}\beta - 9\gamma & -18 + 9\alpha + \frac{9}{2}\beta + 9\gamma & \frac{9}{2} - 9\alpha - \frac{9}{4}\beta \\
y_1 & 3 + 2\alpha - \frac{1}{2}\beta - 2\gamma & \beta & -1 - 2\alpha - \frac{1}{2}\beta + 2\gamma \\
y_2 & \alpha & 1 - \alpha - \gamma & \gamma \\
\hline
 & \boldsymbol{C}(y_0) & \boldsymbol{C}(y_1) & \boldsymbol{C}(y_2)
\end{array},
$$

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

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Derivation of method

Coefficients for the fourth order method (**BDF4-CF**)

$$
\begin{array}{c|cccc}
y_0 & a_{11} & a_{12} & \gamma & \kappa \\
y_1 & a_{21} & a_{22} & a_{23} & a_{24} \\
y_2 & \alpha & a_{32} & \sigma & \varrho \\
y_3 & \beta & a_{42} & a_{43} & a_{44} \\
\hline
 & \boldsymbol{C}(y_0) & \boldsymbol{C}(y_1) & \boldsymbol{C}(y_2) & \boldsymbol{C}(y_3)
\end{array}
$$

with parameters $\alpha, \beta, \gamma, \varrho, \sigma, \kappa \in \mathbb{R}$.

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Derivation of method

where

$$
\begin{aligned}
a_{11} &= 4\alpha - 4\sigma - 8\varrho + 12 + \gamma + 2\kappa,\\
a_{12} &= -4\alpha + 8\varrho - 2\gamma - 3\kappa - 8 + 4\sigma,\\
a_{21} &= -3\beta + 3\alpha - \frac{3}{2}\varrho + \frac{3}{16}\gamma + \frac{3}{8}\kappa - \frac{3}{4}\sigma + \frac{3}{2},\\
a_{22} &= 9\beta - \frac{9}{2}\alpha - \frac{9}{8}\varrho - \frac{9}{32}\gamma - \frac{9}{32}\kappa - \frac{9}{8}\sigma + \frac{21}{4},\\
a_{32} &= 2 - \varrho - \sigma - \alpha,
\end{aligned}
$$

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Derivation of method

where

$$
\begin{aligned}
a_{42} &= \frac{1}{4} - 3\beta + \frac{1}{2}\alpha + \frac{1}{8}\varrho - \frac{3}{32}\kappa - \frac{1}{32}\gamma - \frac{1}{8}\sigma, \\
a_{23} &= -9\beta + \frac{9}{4}\alpha + \frac{9}{4}\varrho - \frac{9}{16}\kappa + \frac{9}{4}\sigma - \frac{9}{2}, \\
a_{24} &= \frac{3}{8}\varrho + 3\beta - \frac{3}{4}\alpha + \frac{3}{32}\gamma + \frac{15}{32}\kappa - \frac{3}{8}\sigma + \frac{3}{4}, \\
a_{43} &= 3\beta - \frac{3}{4}\alpha - \frac{3}{4}\varrho + \frac{1}{16}\gamma + \frac{3}{16}\kappa, \\
a_{44} &= -\beta + \frac{1}{4}\alpha + \frac{5}{8}\varrho - \frac{1}{32}\gamma - \frac{3}{32}\kappa + \frac{1}{8}\sigma + \frac{3}{4}.
\end{aligned}
$$

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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

$$\dot{y} = (\lambda + \hat{\imath}\upsilon)y, \tag{14}$$

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

— 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.

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

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

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

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LINEAR STABILITY

The characteristic polynomials of the **SBDF** methods of [Ascher *et al.*, 1995] and those of BDF-CF 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	$\left(\frac{25}{11}-\omega_R\right)\tau^4 - 4(1+\hat{\imath}\omega_I)\tau^3 + 3(1+2\hat{\imath}\omega_I)\tau^2 - \frac{4}{3}(1+3\hat{\imath}\omega_I) + \frac{1}{4}(1+4\hat{\imath}\omega_I)$

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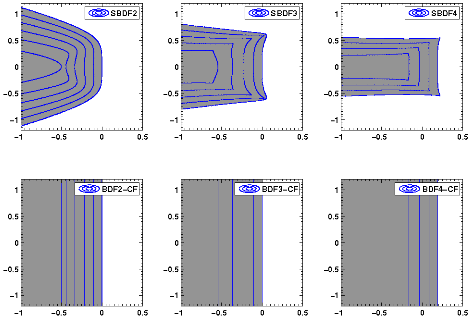
LINEAR STABILITY



Stability domains $\mathcal{S} \subset \mathbb{C}$ (shaded) for SBDF and BDF-CF methods.

Nonlinear test problem

We consider the Burgers equation in $1D$

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

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

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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_∞ grid-norm is measured at time $T = 2$ as a function of viscosity, $0.001 \leqslant \nu \leqslant 0.1$.
- The reference or "exact" solution is computed for $N = 80$ spatial nodes using MATLABs build-in `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

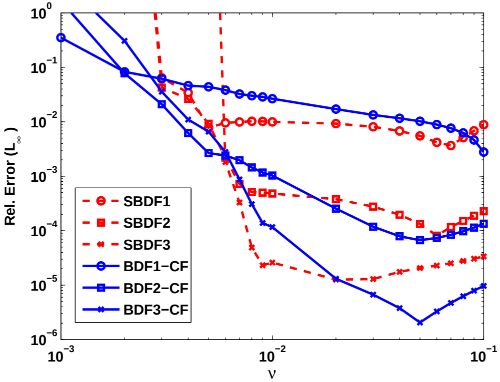

Figure: $h = 1/80$

Nonlinear test problem

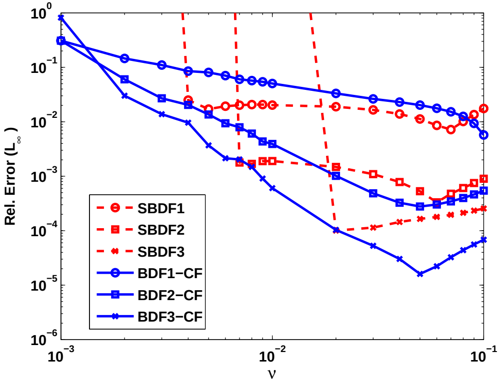

FIGURE: $h = 1/40$

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Nonlinear test problem

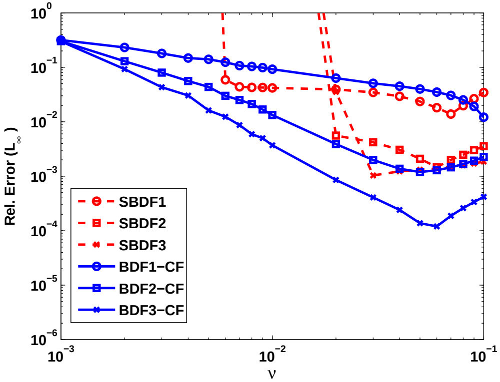

Figure: $h = 1/20$

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Nonlinear test problem

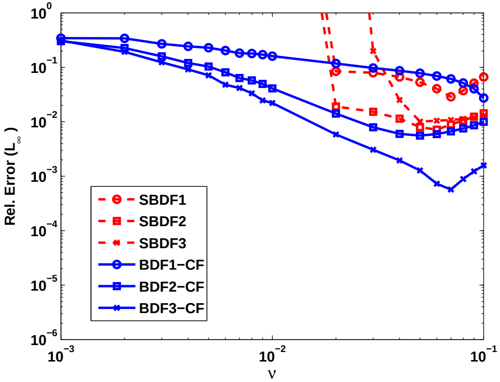

Figure: $h = 1/10$

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Nonlinear test problem- Obseravations

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 $\varphi y = y + \mathcal{O}(h)$.

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

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A SIMPLE TEST CASE

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

$$\begin{aligned} \dot{y}_1 &= y_1^2 + z + \cos t - 1, \\ \dot{y}_2 &= y_1^2 + y_2^2 - \sin t - 1, \quad t \in [1, 2], \\ 0 &= y_1^2 + y_2^2 - 1, \end{aligned} \tag{16}$$

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:

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

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A SIMPLE TEST CASE

- Methods: BDF1-CF, BDF2-CF ($\gamma = 0$), BDF3-CF ($\alpha = \beta = \gamma = 0$) and BDF4-CF ($\alpha = \beta = \gamma = \sigma = \varrho = \kappa = 0$).
- 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 $h = 1/2^r, \ r = 4, \ldots, 11$.

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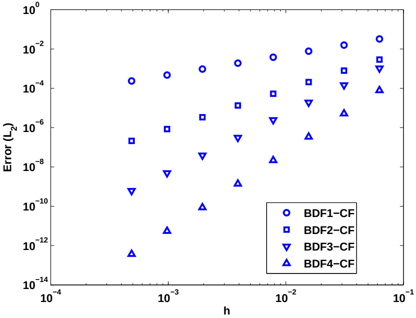
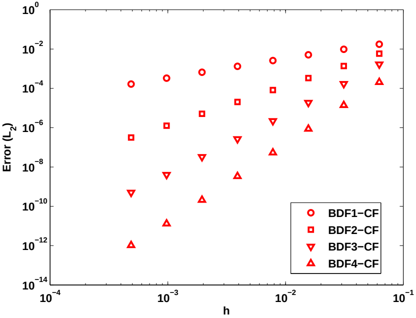
A simple test case



Error in *y*



Error in *z*

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Numerical test on Navier-Stokes

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

$$\begin{aligned} \boldsymbol{u}_t + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} &= -\nabla\bar{p} + \frac{1}{Re}\nabla^2\boldsymbol{u} \quad \text{in} \quad \Omega\times(0,T], \qquad (17)\\ \nabla\cdot\boldsymbol{u} &= 0 \quad \text{in} \quad \Omega\times(0,T], \qquad (18) \end{aligned}$$

with prescribed initial data and velocity boundary conditions.

$Re =$ Reynolds number,
$\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{x},t) = [u_1,u_2]^T \in \mathbb{R}^2$ is the fluid velocity and
$\bar{p} = \bar{p}(\boldsymbol{x},t) \in \mathbb{R}$ is the pressure,
$\boldsymbol{x} = (x_1,x_2) \in \Omega \subset \mathbb{R}^2,\ t \in [0,T],$.

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Numerical test on Navier-Stokes

For the spatial discretization [Fischer et al.2002]

- Spectral element method (SEM) based on a standard Galerkin weak formulation
- $\mathbb{P}_N - \mathbb{P}_{N-2}$ compartible velocity-pressure discrete spaces
- Gauss-Lobatto-Legendre (GLL) nodes for velocity
- Gauss-Legendre (GL) nodes for pressure
- Dirichlet boundary conditions on the spatial domain $\Omega = [-1, 1]^2$

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Numerical test on Navier-Stokes

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

$$\mathbf{B}\dot{y} + \mathbf{C}(y)y + \mathbf{A}y - \mathbf{D}^T z = 0, \quad (19)$$

$$\mathbf{D}y = 0 \quad (20)$$

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 $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}, \mathbf{D}^T$ represent the discrete Poisson (negative Laplace), mass, convection, divergence and gradient operators respectively.

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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

$$\boldsymbol{u} = \begin{bmatrix} -\cos(\pi x_1)\sin(\pi x_2) \\ \sin(\pi x_1)\cos(\pi x_2) \end{bmatrix} \exp(-2\pi^2 t/Re), \tag{21}$$

$$\bar{p} = -\frac{1}{4}(\cos(2\pi x_1) + \cos(2\pi x_2))\exp(-4\pi^2 t/Re), \tag{22}$$

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Numerical test on Navier-Stokes

- Methods: BDF1-CF, BDF2-CF (with $\gamma = 0$) and BDF3-CF (with $\alpha = \beta = \gamma = 0$)
- 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
- $Re = 2\pi^2.$

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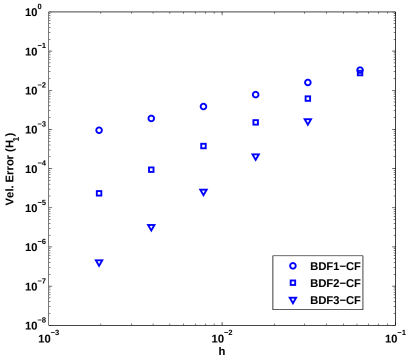
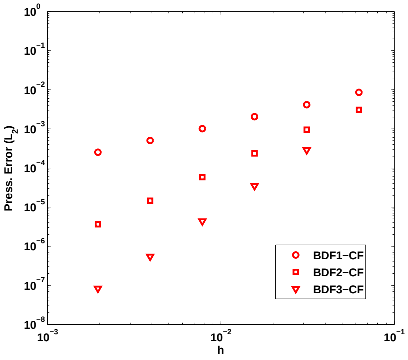
Numerical test on Navier-Stokes



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!**

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