Semi-Lagrangian methods: high order discretizations in space and time

Elena Celledoni

Department of Mathematical Sciences, NTNU, Norway
joint work with B.K Kometa

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Outline

1. Convection diffusion problems
    - Model problem
    - Semi-Lagrangian methods beyond nominal CFL restrictions

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   - Commutator free methods
   - Semi-Lagrangian exponential integrators of RK type
   - Order analysis and examples
   - Semi-Lagrangian exponential integrators of BDF type
   - Examples

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   - Semi-Lagrangian exponential integrators of BDF type
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3. Application to the Navier-Stokes equations
4. Conclusions

Introduction

The model problem: convection and diffusion

- **Convection-diffusion**

$$\frac{\partial}{\partial t}u(\mathbf{x},t) + \mathbf{V}\cdot\nabla u(\mathbf{x},t) = \nu\nabla^2 u + f(\mathbf{x}),$$

with $\mathbf{x} \in \Omega \subset \mathbf{R}^d$ and $\mathbf{V} : \mathbf{R}^d \times [0,T] \to \mathbf{R}^d$ is a vector field, $u : \mathbf{R}^d \times [0,T] \to \mathbf{R}^d$, and $u(\mathbf{x},0) = u_0(\mathbf{x})$. The convecting vector field can also be $\mathbf{V} = u$.

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$$y_t - C(v)y = Ay, \qquad y(0) = y_0,$$

and can be $v = y$. Here C is the discretized convection operator, A corresponds to the linear diffusion term, often negative definite.

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- **Convection dominated problems**: viscosity coefficients are of the order of the mesh size.
- **incompressible Navier-Stokes**

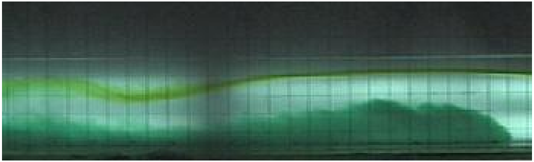
$$\begin{aligned}\frac{\partial\mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u} &= \nu\nabla^2\mathbf{u}-\frac{1}{\rho}\nabla p\\ \nabla\cdot\mathbf{u} &= 0\end{aligned}$$

Fluids with small density variations: Navier-Stokes + Boussinesq approximation

$$\begin{aligned}
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} &= \nu \nabla^2 \mathbf{u} - \frac{1}{\rho} \nabla p + \mathbf{g} \beta \Delta S \\
\nabla \cdot \mathbf{u} &= 0 \\
\frac{\partial S}{\partial t} + \mathbf{u} \cdot \nabla S &= \alpha \nabla^2 S
\end{aligned}$$

Unknowns: velocity, pressure, salinity

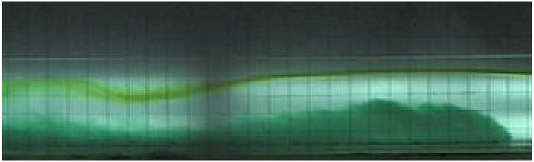
Waves occurring at the interface between two layers of a stratified flow which do not affect the surface.



Internal wave created in a laboratory

What are internal waves?

Waves occurring at the interface between two layers of a stratified flow which do not affect the surface.



Internal wave created in a laboratory

- Such waves influence the ecosystem in fjords.
- Weather prediction influenced by the topography.

- High order space discretizations (numerical dispersion).
- Succesful simulations using a turbulence k-ϵ model.

Need for good integrators for convection dominated problems: IMEX

Consider $y_t - C(v)y = Ay, \quad y(0) = y_0,$ and the method

$$y_{n+1} = y_n + hC(y_n)y_n + hAy_{n+1}$$

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- In time

$$h_{\mathrm{CFL}} \cdot \mathrm{Re}^{\frac{3}{4}\alpha - \frac{1}{2}} \approx \tau$$

  where τ Kolmogorov temporal scale and $\alpha = 1, 3/2, 2$

(Karniadakis et al. 2001, 2006)

A simple improvement

We consider a first order integrator for

$$y_t - C(y)y = Ay, \qquad y(0) = y_0.$$

Example

$$y_{n+1} = \exp(hC(y_n))y_n + hAy_{n+1}.$$

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The exponential $\exp(\gamma hC(w)) \cdot g$ is the solution of the semidiscretized equation

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which corresponds to the pure convection problem

$$\gamma_t + \mathbf{V} \cdot \nabla\gamma = 0, \qquad \gamma(x_i, 0) = g_i, \quad \text{in } [0, h] \times \Omega,$$

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$$\frac{D\gamma}{Dt} = 0, \qquad \gamma(x_i, 0) = g_i, \quad \text{in } [0, h] \times \Omega,$$

The corresponding transport diffusion algorithm

Keeping in mind $y_{n+1} = \exp(hC(y_n))y_n + hAy_{n+1}$.

Transport-diffusion: Pirroneau '82

$$
\begin{aligned}
\frac{Du_{n+\frac{1}{2}}}{Dt} &= 0, \quad u_{n+\frac{1}{2}}(x, t_n) = u_n(x), \quad \text{on } [t_n, t_n + h] \\
& \qquad u_{n+\frac{1}{2}}(x) = u_{n+\frac{1}{2}}(x, t_n + h) \\
u_{n+1} &= u_{n+\frac{1}{2}} + h\nu\nabla^2 u_{n+1},
\end{aligned}
$$

the convecting vector field is $\mathbf{V}(x) = u_n(x)$.

The exact integration of the pure convection problem can be obtained by introducing characteristics,

$$
\begin{aligned}
& u_{n+\frac{1}{2}}(x) = u_{n+\frac{1}{2}}(x, t_n + h) = u_n(X(t_n)) \\
& \frac{dX}{d\tau} = u_n(X(\tau)), \quad X(t_n + h) = x,
\end{aligned}
$$

Semi-Lagrangian methods

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- Semi-Lagrangian methods combined with high order space discretizations lead to **reduced dispersion error**
- combine high order in space with higher order in time and allow **bigger time steps** overcoming nomial CFL restrictions.

Space discretization: spectral element method

- Spectral-Galerkin on $G = \{(x_i^k, x_j^k)^T, i, j = 0, \ldots, p, \quad k = 0, \ldots, Ne\}$ on the square, Gauss-Lobatto-Legendre nodes

$$u^p(\mathbf{x}, t) = \sum_{k=0}^{Ne} \sum_{m=0}^{p} \sum_{n=0}^{p} u_{m,n}^k(t) l_m^k(x) l_n^k(y), \ \ \mathbf{x} = (x, y)^T,$$

$u_{m,n}^k(t) \approx u(x_m^k, x_n^k, t)$ **tensor product basis** of Lagrange basis functions:

$$l_i^k(x) = \prod_{j=0, j\neq i}^{p} \frac{x - x_j^k}{x_i^k - x_j^k}.$$

- piecewise polynomial approximations

Incompressible Navier-Stokes: "thin" shear-layer roll up problem

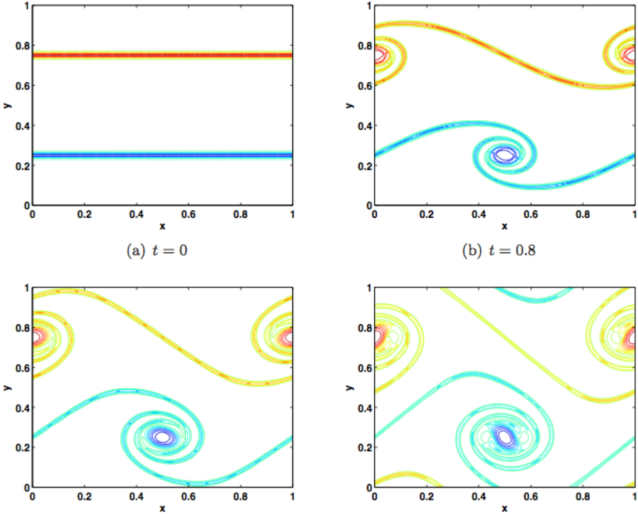
Initial data $\mathbf{u} = (u, v)$

$$u = \begin{cases} \tanh(\rho(y - 0.25)) & \text{for} \quad y \leq 0.5 \\ \tanh(\rho(0.75 - y)) & \text{for} \quad y > 0.5 \end{cases} \qquad v = 0.005 \sin(2\pi x)$$

and layer thickness $\mathcal{O}\left(\frac{1}{\rho}\right)$

- Doubly-periodic BCs on $\Omega = [0, 1]^2$
- spectral element method $Ne = 16 \times 16$, polynomial degree 16
- Filtering procedure: $\alpha = 0.3$: on each element $p_\alpha(x) = \alpha p_N(x) + (1 - \alpha)\tilde{p}_{N-1}(x)$.
- $Re = 10^5$, $h = 0.01$, $Cr \approx 12$
- comparison with Fischer, Kruse and Loth (J. Sci. Comp. 2002), we have 10 times bigger Cr

Incompressible Navier-Stokes: "thin" shear-layer roll up problem



(a) $t = 0$ (b) $t = 0.8$

(c) $t = 1.0$ (d) $t = 1.2$

The integration methods

Commutator-free methods

Let $\mathcal{M}$ be a manifold and consider frame vector fields s.t.

$$T_x\mathcal{M} = \mathrm{span}\{\mathcal{E}_1|_x, \dots \mathcal{E}_d|_x\}, \quad \forall\, x \in \mathcal{M},$$

for any vector field F is s.t.

$$F(y) = \sum_{i=1}^{d} f_i(y)\mathcal{E}_i(y), \quad \text{and} \quad F_p(x) := \sum_{i=1}^{d} f_i(p)\mathcal{E}_i(x)$$

where F_p is the vector field *frozen* at p.

Commutator-free method for $\dot{y} = F(y)$, $y(t_0) = y_0$:

$p = y_n$
for $r = 1 : s$ do

$$Y_r = \exp(\textstyle\sum_{k=1}^{r-1} \alpha_{rJ}^k F_k) \cdots \exp(\sum_{k=1}^{r-1} \alpha_{r1}^k F_k)(p)$$

$$F_r = hF_{Y_r} = h\textstyle\sum_{i=1}^{d} f_i(Y_r)\mathcal{E}_i$$

end

$$y_{n+1} = \exp(\textstyle\sum_{k=1}^{s} \beta_J^k F_k) \cdots \exp(\sum_{k=1}^{s} \beta_1^k F_k)p$$

(Celledoni, Marthinsen, Owren, 2003 FGCS)

In particular if

$$\dot{y} = C(y)\,y, \quad y(t_0) \in G, \quad C(y) \in \mathfrak{g},$$

then

Commutator-free method for

$$\dot{y} = C(y)\,y, \qquad y(t_0) = y_0$$

$p = y_n$
for $r = 1 : s$ do

$$Y_r = \exp(h \textstyle\sum_{k=1}^{r-1} \alpha_{rJ}^k C_k) \cdots \exp(h \sum_{k=1}^{r-1} \alpha_{r1}^k C_k) p$$

$$C_r = C(Y_r)$$

end

$$y_{n+1} = \exp(h \textstyle\sum_{k=1}^{s} \beta_J^k C_k) \cdots \exp(h \sum_{k=1}^{s} \beta_1^k C_k) p$$

Consider

$$\dot{y} - C(y)y = Ay, \qquad y(0) = y_0.$$

and the change of variables $y = Wz$ where $\dot{W} = C(Wz) \cdot W$ and $W(0) = I$ by differentiation

$$\begin{cases} \dot{W} & = & C(Wz) \cdot W \\ \dot{z} & = & W^{-1}AWz \end{cases}$$

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Explicit Lie Euler + Implicit Euler

$$\begin{cases} W_{n+1} & = & \exp(hC(W_n z_n))\, W_n \\ z_{n+1} & = & z_n + hW_{n+1}^{-1}\, A\, W_{n+1}\, z_{n+1} \end{cases}$$

and setting $y_n = W_n z_n$ and $y_{n+1} = W_{n+1} z_{n+1}$ we get

$$y_{n+1} = \exp(hC(y_n))y_n + hAy_{n+1}$$

A new class of exponential integrators

- High order implicit integration method for z compatible with the CF-method.
- No more than one linear system per stage (DIRK).

$$\dot{y} - C(y)y = Ay, \quad y(0) = y_0,$$

for $i = 1 : s$ do

$$Y_i = \varphi_i y_n + h \sum_{j=1}^{i} a_{i,j} \varphi_i \varphi_j^{-1} A Y_j$$

$$\varphi_i = \exp(h \sum_k \alpha_{iJ}^k C(Y_k)) \cdots \exp(h \sum_k \alpha_{i1}^k C(Y_k))$$

end

$$y_{n+1} = \varphi_{s+1} y_n + h \sum_{i=1}^{s} b_i \varphi_{s+1} \varphi_i^{-1} A Y_i$$

$$\varphi_{s+1} = \exp(h \sum_k \beta_J^k C(Y_k)) \cdots \exp(h \sum_k \beta_1^k C(Y_k))$$

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Classical order conditions for the new methods

Assume that $\sum_{l=1}^{J} \alpha_{il}^{j} = \hat{a}_{i,j}$ for $i = 1, \ldots, s$ and $j = 1, \ldots, s$, and that $\sum_{l=1}^{J} \beta_{l}^{j} = \hat{b}_j$.

$$\begin{array}{c|c} \mathbf{c} & A \\ \hline & \mathbf{b} \end{array} \qquad \begin{array}{c|c} \hat{\mathbf{c}} & \hat{A} \\ \hline & \hat{\mathbf{b}} \end{array}$$

Simplifying condition $c_i = \hat{c}_i$.

Order 1 og 2 conditions

	$\|\tau\|-1$	Tree	$F(\tau)$	$\gamma(\tau)$		$\sigma(\tau)$
1	1		C	1	$\sum_i \hat{b}_i$	1
1	1		A	1	$\sum_i b_i$	1
2	2		$C'(C)$	2	$\sum_{i,j} \hat{b}_i \hat{a}_{i,j}$	1
2	2		$C'(A)$	2	$\sum_{i,j} \hat{b}_i a_{i,j}$	1
2	2		CA	2	$\sum_{i,j} b_i \hat{a}_{i,j}$	2
2	2		A^2	2	$\sum_{i,j} b_i a_{i,j}$	1

Set $\sum_{l=1}^{J} \alpha_{il}^{j} = \hat{a}_{i,j}$ for $i = 1, \ldots, s$ and $j = 1, \ldots, s$, and $\sum_{l=1}^{J} \beta_l^j = \hat{b}_j$.

- Order two conditions are the same as the conditions of order two for the PRK method defined by (A, b, c) and $(\hat{A}, \hat{b}, \hat{c})$

Examples of methods

- Any couple of classical RK methods of order 1 give a method of order 1
- A couple of partitioned RK methods of order 2 give a new method of order 2
- We take a pair of PRK of order 3 or 4 (explicit + implicit) and construct a Commutator Free method out of the explicit method s. t.

$$\hat{b}_k = \sum_{l=0}^{J-l} \beta^k_{J-l}, \quad \hat{a}_{k,j} = \sum_{l=0}^{J-l} \alpha^j_{J-l,k}$$

  the resulting method satisfies the conditions for order 3 for the new class of methods.
- Order four involves new coupling conditions.

Order 2

Example

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

$$\begin{aligned} \varphi_{\frac{1}{2}} &= \exp(\tfrac{h}{2} C(y_0)) & Y_{\frac{1}{2}} &= \varphi_{\frac{1}{2}} y_0 + \tfrac{h}{2} A Y_{\frac{1}{2}} \\ \varphi_1 &= \exp(\tfrac{h}{2} C(Y_{\frac{1}{2}})) & y_1 &= \varphi_1 y_0 + h \varphi_1 \varphi_{\frac{1}{2}}^{-1} A Y_{\frac{1}{2}} \end{aligned}$$

Can be written as a **transport-diffusion** method.

Example

Partitioned RK:

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{2}{3} \end{array} \qquad \begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{2} & -\frac{\beta}{2} & \frac{1+\beta}{2} & \\ 1 & \frac{3+5\beta}{2} & -(1+3\beta) & \frac{1+\beta}{2} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{2}{3} \end{array}$$

with $\beta = \frac{\sqrt{3}}{3}$, Griepentrog '78.

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{1}{12} & \frac{1}{3} & -\frac{1}{4} \\ \hline & \frac{1}{12} & \frac{1}{3} & \frac{5}{12} \end{array} \qquad \begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{2} & -\frac{\beta}{2} & \frac{1+\beta}{2} & \\ 1 & \frac{3+5\beta}{2} & -(1+3\beta) & \frac{1+\beta}{2} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{2}{3} \end{array}$$

BDF-CF method: applicable to DAEs

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

BDF-CF method

for $n = k-1 : K-1$ do

$$\varphi_i = \exp(h \textstyle\sum_{j=1}^{k} a_{i+1,j} C(y_{n-k+j})), \quad i = 0, \dots, k-1,$$

$$\alpha_k \, y_{n+1} + \textstyle\sum_{i=0}^{k-1} \alpha_i \, \varphi_i \, y_{n+1-k+i} = hf(y_{n+1}, z_{n+1}),$$

$$0 = g(y_{n+1})$$

end

- IMEX counterpart:SBDFS by Asher et al.
- Relation to the *Operator integrating factor splitting method* by Maday, Patera and Rønquist.
- Relation to SL methods proposed by Xiu and Karniadakis.

A-stability

Improved stability properties compared to the IMEX counterparts.
We consider the test equation:

$$\dot{y} = \lambda y + \hat{i}\mu y,$$

$z := v + \hat{i}w$ where $v = \lambda h$ and $w = \mu h$.

- For the RK-type methods: the A-stability is determined by the stability of the DIRK method with stability function $\tilde{R}(v)$.
  Stability function:

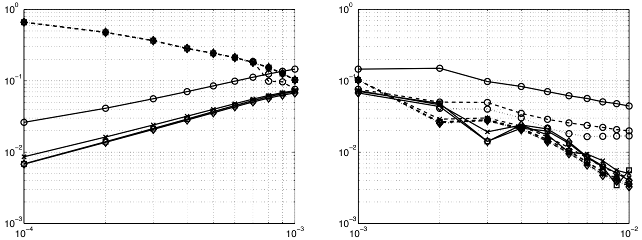
  $$R(v, w) = e^{\hat{i}w}\tilde{R}(v)$$

  IMEX counterpart

  $$R(v, w) := 1 + (v\mathbf{b}^T + \hat{i}w\hat{\mathbf{b}}^T)(I_s - v\mathcal{A} - \hat{i}w\hat{\mathcal{A}})^{-1}\mathbf{1}_s,$$

- Similarly for the BDF-CF vs SBDF.

Viscous Burgers equation: $u_t + uu_x = \nu u_{xx}$



$\nu \in [10^{-4}, 10^{-3}]$ $\nu \in [10^{-3}, 10^{-2}]$

- $u(x,0) = \sin(\pi x)$, fixed $\Delta x = 1/81$, $t = 2$, $h = 1.8\Delta x$;
- plot: viscosity ν on the x-axis relative error y-axis
- time integrators: IMEX (dotted line), DIRK-CF (dashed line) and SL DIRK-CF (solid line);
- finite differences with piecewise cubic monotonic interpolation;
- Symbols: (o) order 1; (x) order 2, (+) order 2 of type L; diamonds order 3 and squares order 3 type G.
- the characteristic velocity $U \leq 1$ the Peclet number is $Pe \leq \frac{1}{81\nu}$ and the Courant number is 1.8.

Application to the Navier-Stokes equations, the one step case

- Semidiscretization and BCs
- semi-Lagrangian implementation
- Joint work with Kometa and Verdier

Navier-Stokes equations, space discretization

$$\begin{aligned} \frac{\partial}{\partial t}\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} &= \nu\nabla^2\mathbf{u} - \frac{1}{\rho}\nabla p \\ \nabla\cdot\mathbf{u} &= 0 \end{aligned}$$

- Semidiscretization (SEM) based on Galerkin weak formulation.
- Ne rectangular uniform elements.
- Approximation space: $\mathbb{P}_N - \mathbb{P}_{N-2}$ compatible velocity-pressure discrete spaces: N-degree polynomial for the velocity, $(N-2)$-degree polynomial for the pressure, both based on Gauss-Lobatto-Legendre points.

$$\begin{aligned} \Sigma\dot{y} &= QQ^T A\,y + QQ^T C(y)\,y + QQ^T D^T p, \\ Dy &= 0, \\ y &= Q\bar{y}. \end{aligned}$$

- M: total number of degrees of freedom including the boundaries, $y \in \mathbf{R}^M$;
- $k \leq M$: degrees of freedom necessary and sufficient to express the numerical solution: $\bar{y} \in \mathbf{R}^k$; $Q : \mathbf{R}^k \to \mathbf{R}^M$.
- $\Sigma = QQ^T B$, B mass matrix, QQ^T enforces boundary conditions: Σ invertible on the range of Q.

Semi-discrete Navier-Stokes equations

- **Minimal number of degrees of freedom**:

$$\begin{aligned} \bar{B}\dot{\bar{y}} &= \bar{A}\,\bar{y} + \bar{C}(\bar{y})\,\bar{y} + \bar{D}^T p, \\ \bar{D}\bar{y} &= 0, \end{aligned}$$

$\bar{B} = Q^T BQ$, $\bar{A} = Q^T AQ$, $\bar{C}(\bar{y}) = Q^T C(Q\bar{y})\,Q$ and $\bar{D} = DQ$.

- **Projected equations**

$$\dot{\bar{y}} = \bar{\Pi}\bar{B}^{-1}(\bar{A}\,\bar{y} + \bar{C}(\bar{y})\,\bar{y}).$$

$\bar{\Pi} = I - \bar{H}$ and $\bar{H} := \bar{B}^{-1}\bar{D}^T(\bar{D}\bar{B}^{-1}\bar{D}^T)^{-1}\bar{D}$.

for $i = 1 : s$ do

$\quad \bar{Y}_i = \varphi_i \bar{y}_n + h\sum_{j=1}^{i} a_{i,j}\varphi_i\varphi_j^{-1}\bar{\Pi}\bar{B}^{-1}\bar{A}\bar{Y}_j$

$\quad \bar{Y}_i^\gamma := \sum_k \alpha_{i\,\gamma}^k \bar{Y}_k$ for $\gamma = 1, \dots, J$

$\quad \varphi_i = \exp(h\bar{\Pi}\bar{B}^{-1}\bar{C}(\bar{Y}_i^J)) \cdots \exp(h\bar{\Pi}\bar{B}^{-1}\bar{C}(\bar{Y}_i^1))$

end

$\bar{y}_{n+1} = \varphi_{s+1}\bar{y}_n + h\sum_{i=1}^{s} b_i\varphi_{s+1}\varphi_i^{-1}\bar{\Pi}\bar{B}^{-1}\bar{A}\bar{Y}_i, \quad y_{n+1} = Q\bar{y}_{n+1}$

$\bar{Y}_{s+1}^\gamma := \sum_k \beta_\gamma^k \bar{Y}_k$ for $\gamma = 1, \dots, J$

$\varphi_{s+1} = \exp(h\bar{\Pi}\bar{B}^{-1}\bar{C}(\bar{Y}_{s+1}^J)) \cdots \exp(h\bar{\Pi}\bar{B}^{-1}\bar{C}(\bar{Y}_{s+1}^1))$

Semi-Lagrangian implementation

The exponential $\exp(h\bar{\Pi}\bar{B}^{-1}\bar{C}(\bar{w}))\cdot g$ is the solution of the semidiscretized equation

$$\begin{aligned}\bar{B}\dot{\bar{v}} &= \bar{C}(\bar{w})\,\bar{v}+\bar{D}^T p,\\ \bar{D}\bar{v} &= 0, \qquad\qquad [0,h],\end{aligned}$$

which corresponds to a set of *linearized* Euler equations

$$\gamma_t+\mathbf{V}\cdot\nabla\gamma=\nabla p,\qquad \gamma(x_i,0)=g_i,\quad \text{in } [0,h]\times\Omega,$$
$$\nabla\cdot\gamma=0,$$

Options:

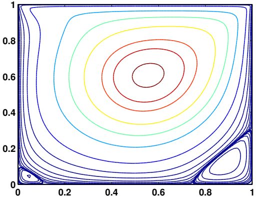
- Use a projection method of high order for γ:

$$\exp(h\bar{\Pi}\bar{B}^{-1}\bar{C}(\bar{w}))\cdot g=\bar{\Pi}\exp(h\bar{B}^{-1}\bar{C}(\bar{w}))\cdot g+\bar{\Pi}E$$

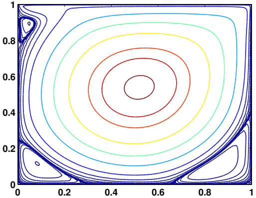
- Consider the vorticity formulation: $\omega_t+\mathbf{V}\cdot\nabla\omega+f(\omega)=0$ and $\omega=\nabla\times\gamma$.

Lid-driven cavity flow, 2D

- $u = 1$ on upper portion of $\partial\Omega$, $u = 0$ elsewere.
- $Ne = 10$, $N = 10$.
- $\Delta t = 0.03$, $Cr = 9.0911$.



$Re = 400$



$Re = 3200$

CONCLUSIONS

Summary

- So far we wanted to verify that the approach works and really allows larger time steps for convection dominated problems.
- This depends also on a number of smart choices in the implementation.

Future work

- Implementation issues (projections). Lots of possible improvements.
- Convergence analysis both of the Eulerian and the semi-Lagrangian case.

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Thanks

Thanks. . .

for your attention!