Eulerian and Semi-Lagrangian exponential integrators for convection dominated problems

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   • Semidiscretized equations
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   - Semidiscretized equations
   - Numerical dispersion

2. Time integrators and transport diffusion algorithms
   - Curing numerical dispersion by computing characteristics
   - Integrating factor like methods
   - Partitioned RK-CF methods
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3. Numerical tests
Outline

1. Convection diffusion problems
   - Semidiscretized equations
   - Numerical dispersion

2. Time integrators and transport diffusion algorithms
   - Curing numerical dispersion by computing characteristics
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   - Partitioned RK-CF methods

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Introduction
Consider

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

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

\[
y_t - C(v)y = Ay + f, \quad y(0) = y_0,
\]

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

Example

A linear convection diffusion problem in 1D

\[
\frac{\partial}{\partial t} u + \frac{\partial}{\partial x} u = \nu \nabla^2 u + f, \quad f = 1
\]

\(u(x, 0) = \cos(x \pi / 2)\) and homogeneous Dirichlet BCs.

We discretize in space with spectral Galerking methods and integrate in time with an implicit-explicit order 3 method.
Numerical dispersion with spectral element methods

\( \nu = 0.01, \ K = 1, \ p = 16 \)

\( \nu = 0.001, \ K = 1, \ p = 32 \)
A simple method

We consider a first order integrator for

$$y_t - C(y)y = Ay + f, \quad y(0) = y_0.$$  

Example

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

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

\[ v' = C(w)v, \quad v(0) = g, \quad \text{in } [0, h], \]
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Example

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\[ v' = C(w)v, \quad v(0) = g, \quad \text{in } [0, h], \]

which corresponds to the pure convection problem

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

\[ \frac{D\gamma}{Dt} = 0, \quad \gamma(x_i, 0) = g_i, \quad \text{in } [0, h] \times \Omega, \]
The corresponding transport diffusion algorithm

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

**Transport-diffusion: Pirroneau ’82**

\[
\frac{Du_{n+\frac{1}{2}}}{Dt} = 0, \quad u_{n+\frac{1}{2}}(x, t_n) = u_n(x), \quad \text{on } [t_n, t_n + h]
\]

\[
u_{n+\frac{1}{2}}(x) = u_{n+\frac{1}{2}}(x, t_n + h)
\]

\[
u_{n+1} = u_{n+\frac{1}{2}} + h\nu\nabla^2 u_{n+1} + hf,
\]

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,

\[
u_{n+\frac{1}{2}}(x) = u_{n+\frac{1}{2}}(x, t_n + h) = u_n(X(t_n))
\]

\[
\frac{dX}{d\tau} = u_n(X(\tau)), \quad X(t_n + h) = x,
\]
Numerical tests with semi-Lagrangian spectral element methods

\[ u(x,10) \]

\[ \nu = 0.01, \ K = 1, \ p = 16 \quad \text{and} \quad \nu = 0.001, \ K = 1, \ p = 32 \]

(Celledoni 2003)
The integration methods
Consider

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

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

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

**Explicit Lie Euler + Implicit Euler**

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

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

$$y_{n+1} = \exp(hC(y_n))y_n + hAy_{n+1}$$
Integrating factor methods for nonlinear CD problems

Consider

\[ \dot{y} - C(y)y = Ay, \quad y(0) = y_0, \quad y = Wz \to \begin{cases} \dot{W} = C(Wz) \cdot W \\ \dot{z} = W^{-1}AWz \end{cases} \]

Given \( y_{n-1}, y_n \), consider \( p_1(t) = -\frac{t-t_n}{h}y_{n-1} + \frac{t-t_{n-1}}{h}y_n \)

\[ \begin{cases} \dot{\tilde{W}} = C(p_1(t)) \cdot \tilde{W} \\ \dot{\tilde{z}} = \tilde{W}^{-1}A\tilde{W}\tilde{z} \end{cases}, \quad \text{on } [t_{n-1}, t_n] \]

apply BDF2 for \( \tilde{z} \), and find 'accurately' \( \tilde{W}(t) \),

\[ \frac{3}{2} \tilde{z}_{n+1} = 2\tilde{z}_n - \frac{1}{2} \tilde{z}_{n-1} + h\tilde{W}(t_{n+1})^{-1}A\tilde{W}(t_{n+1})\tilde{z}_{n+1} \]

set \( y_n = \tilde{W}_n\tilde{z}_n, \quad y_{n+1} = \tilde{W}(t_{n+1})\tilde{z}_{n+1} \)

\[ \frac{3}{2} y_{n+1} = 2\tilde{W}(h)y_n - \frac{1}{2} \tilde{W}(2h)y_{n-1} + hAy_{n+1} \]
Consider

\[ \dot{y} - C(y)y = Ay, \quad y(0) = y_0, \quad y = Wz \rightarrow \begin{cases} \dot{W} &= C(Wz) \cdot W \\ \dot{z} &= W^{-1}AWz \end{cases} \]

Interpolate \((t_{n-2}, y_{n-2}), (t_{n-1}, y_{n-1}), (t_n, y_n), \) with \(p_2(t)\)

\[
\begin{cases}
\dot{\tilde{W}} &= C(p_2(t)) \cdot \tilde{W} \\
\dot{\tilde{z}} &= \tilde{W}^{-1}A\tilde{W}\tilde{z}
\end{cases}
\]

\[
\frac{11}{6}y_{n+1} = 3\tilde{W}(h)y_n - \frac{3}{2}\tilde{W}(2h)y_{n-1} + \frac{1}{3}\tilde{W}(3h)y_{n-2} + hAy_{n+1}
\]

(Maday, Patera, Rønquist, 1994, Xiu and Karniadakis, 2001)
Keeping in mind

\[ \frac{3}{2} y_{n+1} = 2 \tilde{W}(h)y_n - \frac{1}{2} \tilde{W}(2h)y_{n-1} + hAy_{n+1} \]

**Transport-diffusion**

\[
\begin{align*}
\frac{D\tilde{u}_n}{Dt} &= 0, \quad \tilde{u}_n(x, t_n) = u_n(x), \quad \text{on } [t_n, t_n + h] \\
\tilde{u}_n(x) &= \tilde{u}_n(x, t_n + h) \\
\frac{D\tilde{u}_{n-1}}{Dt} &= 0, \quad \tilde{u}_{n-1}(x, t_{n-1}) = u_{n-1}(x), \quad \text{on } [t_{n-1}, t_n + h] \\
\tilde{u}_{n-1}(x) &= \tilde{u}_{n-1}(x, t_n + h) \\
\frac{3}{2} u_{n+1} &= 2\tilde{u}_n - \frac{1}{2} \tilde{u}_{n-1} + h\nu \nabla^2 u_{n+1},
\end{align*}
\]

the convecting vector field is

\[ \mathbf{V}(x, t) = -\frac{t-t_n}{h} u_{n-1}(x) + \frac{t-t_{n-1}}{h} u_n(x). \]
In the case of convection diffusion problems, they naturally correspond to a transport-diffusion method.

- Require only one linear system per step
- Good stability properties

- Need a Runge-Kutta method to start
- Linearize the equations via extrapolation
\[ \dot{y} - C(y)y = Ay, \quad y(0) = y_0, \quad y = Wz \rightarrow \left\{ \begin{array}{ll} \dot{W} & = C(Wz) \cdot W \\\n\dot{z} & = W^{-1}AWz \end{array} \right. \]

for \( i = 1 : s \) do

\[ Z_i = z_n + h \sum_{j=1}^{i} a_{i,j} Q_j^{-1} AQ_j Z_j \]

\[ Q_i = \exp(h \sum_{k} \alpha_{i,j}^k C(Q_k Z_k)) \cdots \exp(h \sum_{k} \alpha_{i,1}^k C(Q_k Z_k)) \cdot W_n \]

end

\[ z_{n+1} = z_n + h \sum_{i=1}^{s} b_i Q_i^{-1} AQ_i Z_i \]

\[ W_{n+1} = \exp(h \sum_{k} \beta_{j}^k C(Q_k Z_k)) \cdots \exp(h \sum_{k} \beta_{1}^k C(Q_k Z_k)) \cdot W_n \]
By setting \( Y_i = Q_i Z_i \), \( y_{n+1} = W_{n+1} z_{n+1} \) and \( \varphi_{n+1} = W_{n+1} W_n^{-1} \) in the previous algorithm we get a method we apply directly on

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

for \( i = 1 : s \) do

\[
Y_i = \varphi_i y_n + h \sum_{j=1}^{i} a_{i,j} \varphi_i \varphi_j^{-1} AY_j
\]

\[
\varphi_i = \exp(h \sum_k \alpha_{ij}^k C(Y_k)) \cdots \exp(h \sum_k \alpha_{i1}^k C(Y_k))
\]

end

\[
y_{n+1} = \varphi_{n+1} y_n + h \sum_{i=1}^{s} b_i \varphi_{n+1} \varphi_i^{-1} AY_i
\]

\[
\varphi_{n+1} = \exp(h \sum_k \beta_{ij}^k C(Y_k)) \cdots \exp(h \sum_k \beta_{i1}^k C(Y_k))
\]
Order conditions

- for moderate order via Taylor expansion
- in general for Partitioned RK-methods, use P-series (Hairer, Murua ...)
- for Commutator-Free (Owren work in progress)

Assume that \( \sum_{i=1}^{J} \alpha_{i}^{j} = \hat{a}_{i,j} \) for \( i = 1, \ldots, s \) and \( j = 1, \ldots, s \), and that \( \sum_{i=1}^{J} \beta_{i}^{j} = \hat{b}_{j} \). Simplifying condition \( c_i = \hat{c}_i \).

**Necessary condition for order \( p \):** The given method has order \( p \) only if

\[
\begin{array}{c|c|c|c|c}
\text{c} & A & \hat{A} \\
\hline
\text{b} & \hat{b} \\
\end{array}
\]

satisfy the conditions of order \( p \) for partitioned RK-methods. Using this criterion we derived methods up to order three.
\[
\begin{align*}
\varphi_{1/2} & = \exp\left(\frac{h}{2} C(y_0)\right) \quad Y_{1/2} = \varphi_{1/2} y_0 + \frac{h}{2} AY_{1/2} \\
\varphi_1 & = \exp\left(\frac{h}{2} C(Y_{1/2})\right) \quad y_1 = \varphi_1 y_0 + h\varphi_1 \varphi_{1/2}^{-1} AY_{1/2}
\end{align*}
\]
Transport-diffusion algorithm order 2

\[
\frac{D\tilde{u}_0}{Dt} = 0, \quad \tilde{u}_0(x, 0) = u_0(x), \quad \text{on } [0, \frac{h}{2}]
\]
\[\mathbf{V}(x) = u_0(x)\]
\[\tilde{u}_0(x) = \tilde{u}_0(x, \frac{h}{2})\]

\[
u_{\frac{1}{2}} = \tilde{u}_0 + h\nu \nabla^2 u_{\frac{1}{2}},
\]

\[
\frac{D\tilde{u}_{\frac{1}{2}}}{Dt} = 0, \quad \tilde{u}_{\frac{1}{2}}(x, 0) = u_{\frac{1}{2}}(x), \quad \text{on } [-\frac{h}{2}, 0]
\]
\[\mathbf{V}(x) = u_0(x)\]
\[\tilde{u}_{\frac{1}{2}}(x) = \tilde{u}_{\frac{1}{2}}(x, -\frac{h}{2})\]

\[
\frac{Du_1}{Dt} = 0, \quad u_1(x, 0) = \tilde{u}_{\frac{1}{2}}(x), \quad \text{on } [0, h]
\]
\[\mathbf{V}(x) = u_{\frac{1}{2}}(x)\]
\[u_1(x) = u_1(x, h)\]
### Example

**Partitioned RK:**

\[
\begin{array}{c|ccc}
0 & 1 & 2 \\
\frac{1}{2} & \frac{1}{2} & 2 \\
1 & -1 & 2 \\
\hline
\frac{1}{6} & \frac{2}{3} & \frac{2}{3} \\
\end{array}
\quad
\begin{array}{c|ccc}
0 & 0 & 1 + \beta \\
\frac{1}{2} & -\frac{\beta}{2} & 1 + \beta \\
1 & 3 + 5\beta & -1 + 3\beta \\
\hline
\frac{1}{6} & \frac{2}{3} & \frac{2}{3} \\
\end{array}
\]

with \( \beta = \frac{\sqrt{3}}{3} \), Griepentrog '78.
Order 3

Assume $C_i = C(Y_i)$

Example

$\tilde{Y}_1 = [y_0 - h\frac{\beta}{2} Ay_0]$

$Y_1 = (I - \frac{1+\beta}{2} hA)^{-1} \exp(\frac{h}{2} C_0) \tilde{Y}_1$

$\tilde{Y}_2 = [y_0 + h\frac{(3+5\beta)}{2} Ay_0 - h(1 + 3\beta) \exp(-\frac{h}{2} C_0) AY_1]$

$Y_2 = (I - \frac{1+\beta}{2} hA)^{-1} \exp(-hC_0 + 2hC_1) \tilde{Y}_2$

$\tilde{y}_1 = y_0 + \frac{h}{6} Ay_0 + \frac{h^2}{3} \exp(-\frac{h}{2} C_0) AY_1 + \frac{h}{6} \exp(hC_0 - 2hC_1) AY_2$

$y_1 = \exp(\frac{h}{12} C_0 + \frac{h}{3} C_1 + h\frac{5}{12} C_2) \exp(\frac{h}{12} C_0 + h\frac{1}{3} C_1 - h\frac{1}{4} C_2) \tilde{y}_1$
NUMERICAL TESTS
We consider

\[ y' = C(y)y + Ay, \quad y(0) = y_0 \]

Global error at \( t = 1 \)
Viscous Burgers’ equation

We consider

\[ \frac{\partial}{\partial t} u + u \frac{\partial}{\partial x} u = \nu \nabla^2 u \]

\[ u(x, 0) = \frac{1}{2} \sin(x\pi) \] on \([0, 1]\) and homogeneous Dirichlet BCs, integrated on \([0, 2]\), \(h = 1/64\).

\[ \nu = 1/10, \quad K = 50, \quad p = 8 \]
\[ \nu = 0.05, \ K = 1, \ p = 64 \]

\[ \nu = 0.01, \ K = 1, \ p = 64 \]
Viscous Burgers’ equation

We consider

$$\frac{\partial}{\partial t} u + u \frac{\partial}{\partial x} u = \nu \nabla^2 u$$

$$u(x, 0) = \frac{1}{2} \sin(x \pi) + \sin(x 2 \pi)$$ on $[0, 1]$ and homogeneous Dirichlet BCs, integrated on $[0, 2]$, $h = 1/64$.

$$\nu = 0.2, \ K = 1, \ p = 64$$
Future work

- More numerical tests on nonlinear problems should be made
- Complete the study of the order conditions
- Find in this class efficient methods compared to eg. nonlinear integrating factor methods
- Efficient computation of the *exponentials* in the semi-Lagrangian case (Celledoni and Rønquist)
Thanks... for your attention!