Eulerian and Semi-Lagrangian exponential integrators for convection dominated problems

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Outline

1. Convection diffusion problems
    - Semidiscretized equations
    - Numerical dispersion

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    - Partitioned RK-CF methods

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3. Numerical tests

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    - Integrating factor like methods
    - Partitioned RK-CF methods
3. Numerical tests
4. Conclusions

Introduction

The problems

Consider

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

with $\mathbf{x} \in \Omega \subset \mathbb{R}^d$ 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 $u(\mathbf{x}, 0) = u_0(\mathbf{x})$. The convecting vector field can also be $\mathbf{V} = u$. After semidiscretization

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

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

Linear convection diffusion

Example

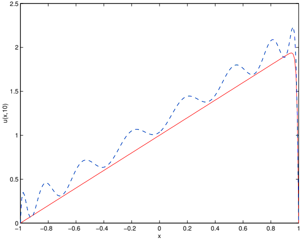
A linear convection diffusion problem in 1D

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

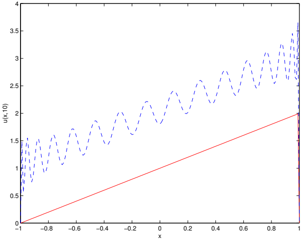
$u(x,0) = \cos(x\pi/2)$ and homogeneous Dirichlet BCs.

We discretize in space with spectral Galerking methods and integrate in time with a 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

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

Example

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

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

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

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

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

which corresponds to the pure convection problem

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

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

The corresponding transport diffusion algorithm

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

Transport-diffusion: Pirroneau '82

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

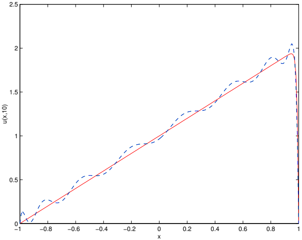
the convecting vector field is $\mathbf{V}(x) = u_n(x)$.

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

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

$$\frac{dX}{d\tau} = u_n(X(\tau)), \quad X(t_n + h) = x,$$

Numerical tests with semi-Lagrangian spectral element methods



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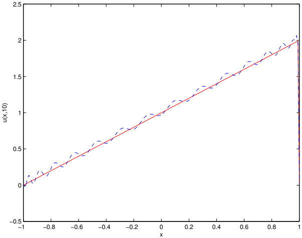


$\nu = 0.001$, $K = 1$, $p = 32$

(Celledoni 2003)

The integration methods

Integrating factor methods for nonlinear CD problems

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

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

Explicit Lie Euler + Implicit Euler

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

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

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

Integrating factor methods for nonlinear CD problems

Consider

$$\dot{y} - C(y)y = Ay, \quad y(0) = y_0, \quad y = Wz \quad \rightarrow \left\{ \begin{array}{rcl} \dot{W} & = & C(Wz) \cdot W \\ \dot{z} & = & W^{-1}AWz \end{array} \right.$$

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

$$\left\{ \begin{array}{rcl} \dot{\tilde{W}} & = & C(p_1(t)) \cdot \tilde{W} \\ \dot{\tilde{z}} & = & \tilde{W}^{-1} A \tilde{W} \tilde{z} \end{array} \right. , \quad \text{on } [t_{n-1}, t_n]$$

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

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

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

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

Integrating factor methods for nonlinear CD problems

Consider

$$\dot{y} - C(y)y = Ay, \quad y(0) = y_0, \quad y = Wz \quad \rightarrow \left\{ \begin{array}{lcl} \dot{W} & = & C(Wz) \cdot W \\ \dot{z} & = & W^{-1}AWz \end{array} \right.$$

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

$$\left\{ \begin{array}{lcl} \dot{\tilde{W}} & = & C(p_2(t)) \cdot \tilde{W} \\ \dot{\tilde{z}} & = & \tilde{W}^{-1}A\tilde{W}\tilde{z} \end{array} \right.$$

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

(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

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

the convecting vector field is
$\mathbf{V}(x,t) = -\frac{t-t_n}{h}u_{n-1}(x) + \frac{t-t_{n-1}}{h}u_n(x)$.

Summarizing for nonlinear integrating factor methods

+ In the case of convection diffusion problems, they naturally correpond 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

Partitioned Runge-Kutta and Commutator-Free

$$\dot{y} - C(y)y = Ay, \quad y(0) = y_0, \quad y = Wz \quad \rightarrow \left\{ \begin{array}{ccc} \dot{W} & = & C(Wz) \cdot W \\ \dot{z} & = & W^{-1}AWz \end{array} \right.$$

```
for $i = 1 : s$ do
    $Z_i = z_n + h \sum_{j=1}^{i} a_{i,j} Q_j^{-1} A Q_j Z_j$
    $Q_i = \exp(h \sum_k \alpha_{iJ}^k C(Q_k Z_k)) \cdots \exp(h \sum_k \alpha_{i1}^k C(Q_k Z_k)) \cdot W_n$
end
$z_{n+1} = z_n + h \sum_{i=1}^{s} b_i Q_i^{-1} A Q_i Z_i$
$W_{n+1} = \exp(h \sum_k \beta_J^k C(Q_k Z_k)) \cdots \exp(h \sum_k \beta_1^k C(Q_k Z_k)) \cdot W_n$
```

DIRK + explicit Commutator-Free

Exponential integrators

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
    $Y_i = \varphi_i y_n + h \sum_{j=1}^{i} a_{i,j} \varphi_i \varphi_j^{-1} A Y_j$
    $\varphi_i = \exp(h \sum_k \alpha_{iJ}^k C(Y_k)) \cdots \exp(h \sum_k \alpha_{i1}^k C(Y_k))$
end
$y_{n+1} = \varphi_{n+1} y_n + h \sum_{i=1}^{s} b_i \varphi_{n+1} \varphi_i^{-1} A Y_i$
$\varphi_{n+1} = \exp(h \sum_k \beta_J^k C(Y_k)) \cdots \exp(h \sum_k \beta_1^k C(Y_k))$
```

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 $\sum_{l=1}^{J} \alpha_{il}^{j} = \hat{a}_{i,j}$ for $i = 1, \dots, s$ and $j = 1, \dots, s$, and that $\sum_{l=1}^{J} \beta_{l}^{j} = \hat{b}_{j}$. Simplifying condition $c_i = \hat{c}_i$.

Necessary condition for order p: The given method has order p only if

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

satisfy the conditions of order p for partitioned RK-methods. Using this criterion we derived methods up to order three.

Order 2

Example

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

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

Transport-diffusion algorithm order 2

$$\begin{aligned}
\frac{D\tilde{u}_0}{Dt} &= 0, \quad \tilde{u}_0(x,0) = u_0(x), \quad \text{on } [0, \tfrac{h}{2}] \\
&\qquad \mathbf{V}(x) = u_0(x) \\
&\qquad \tilde{u}_0(x) = \tilde{u}_0(x, \tfrac{h}{2}) \\
u_{\frac{1}{2}} &= \tilde{u}_0 + h\nu\nabla^2 u_{\frac{1}{2}}, \\
\frac{D\tilde{u}_{\frac{1}{2}}}{Dt} &= 0, \quad \tilde{u}_{\frac{1}{2}}(x,0) = u_{\frac{1}{2}}(x), \quad \text{on } [-\tfrac{h}{2}, 0] \\
&\qquad \mathbf{V}(x) = u_0(x) \\
&\qquad \tilde{u}_{\frac{1}{2}}(x) = \tilde{u}_{\frac{1}{2}}(x, -\tfrac{h}{2}) \\
\frac{Du_1}{Dt} &= 0, \quad u_1(x,0) = \tilde{u}_{\frac{1}{2}}(x), \quad \text{on } [0, h] \\
&\qquad \mathbf{V}(x) = u_{\frac{1}{2}}(x) \\
&\qquad u_1(x) = u_1(x, h)
\end{aligned}$$

Order 3

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.

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

Order 3

Assume $C_i = C(Y_i)$

Example

$$\tilde{Y}_1 = [y_0 - h\tfrac{\beta}{2}Ay_0]$$
$$Y_1 = (I - \tfrac{1+\beta}{2}hA)^{-1}\exp(\tfrac{h}{2}C_0)\tilde{Y}_1$$

$$\tilde{Y}_2 = [y_0 + h\tfrac{(3+5\beta)}{2}Ay_0 - h(1+3\beta)\exp(-\tfrac{h}{2}C_0)AY_1]$$
$$Y_2 = (I - \tfrac{1+\beta}{2}hA)^{-1}\exp(-hC_0 + 2hC_1)\tilde{Y}_2$$

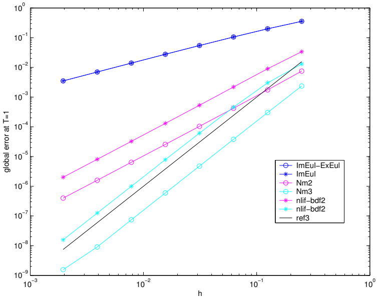
$$\tilde{y}_1 = y_0 + \tfrac{h}{6}Ay_0 + h\tfrac{2}{3}\exp(-\tfrac{h}{2}C_0)AY_1 + \tfrac{h}{6}\exp(hC_0 - 2hC_1)AY_2$$
$$y_1 = \exp(\tfrac{h}{12}C_0 + \tfrac{h}{3}C_1 + h\tfrac{5}{12}C_2)\exp(\tfrac{h}{12}C_0 + \tfrac{h}{3}C_1 - h\tfrac{1}{4}C_2)\tilde{y}_1$$

NUMERICAL TESTS

Order test

We consider

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



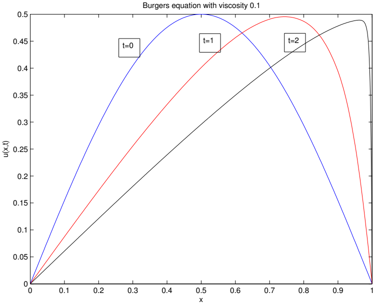
Global error at $t = 1$

Viscous Burgers' equation

We consider

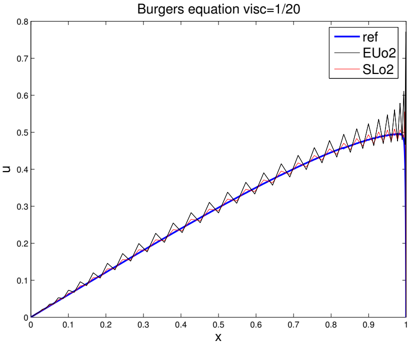
$$\frac{\partial}{\partial t}u + u\frac{\partial}{\partial x}u = \nu\nabla^2 u$$

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

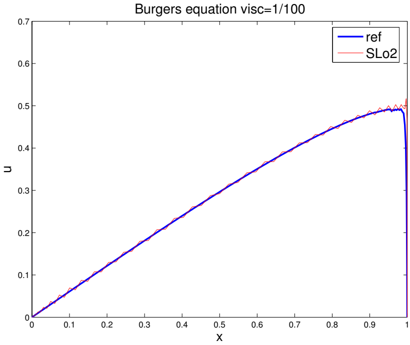


$$\nu = 1/10,\ K = 50,\ p = 8$$

Nonlinear test example



$\nu = 0.05, \; K = 1, \; p = 64$



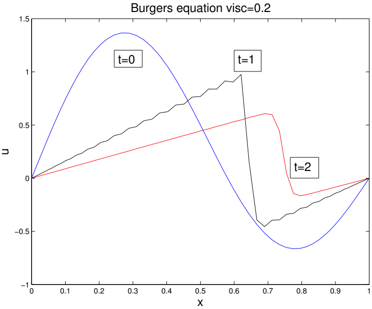
$\nu = 0.01, \; K = 1, \; p = 64$

Viscous Burgers' equation

We consider

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

$u(x,0) = \frac{1}{2}\sin(x\pi) + \sin(x2\pi)$ on $[0,1]$ and homogeneous Dirichlet BCs, integrated on $[0,2]$, $h = 1/64$.



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

CONCLUSIONS

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

Thanks. . .

for your attention!