Eulerian and Semi-Lagrangian exponential integrators for convection dominated problems

Elena Celledoni

Department of Mathematical Sciences, NTNU, Norway

Cambridge, 6th July 2007

Outline

1. Convection diffusion problems
    - Semidiscretized equations
    - Numerical dispersion

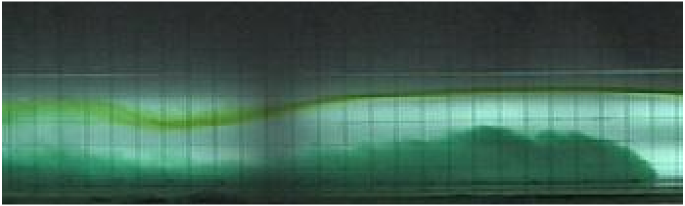
Outline

1. Convection diffusion problems
   - Semidiscretized equations
   - Numerical dispersion
2. Time integrators and transport diffusion algorithms
   - Computing pure convection problems accurately
   - Partitioned RK-CF methods

Outline

1. Convection diffusion problems
   - Semidiscretized equations
   - Numerical dispersion
2. Time integrators and transport diffusion algorithms
   - Computing pure convection problems accurately
   - Partitioned RK-CF methods
3. Numerical tests

Introduction



Navier-Stokes + Boussinesque approximation

Modelling of fluids with small density variations

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

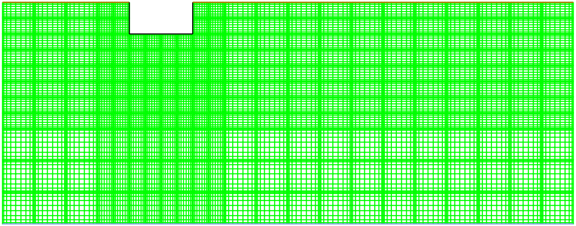
Unknowns:

$\mathbf{u}$	velocity
p	pressure
S	temperature (passive scalar)

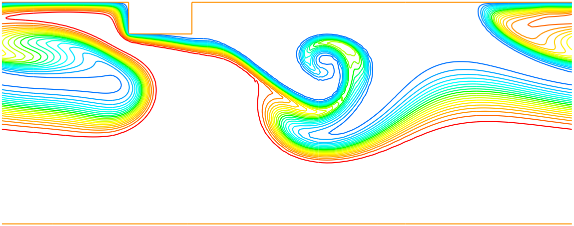
Parameters:

ν	$=$	$\frac{\mu}{\rho}$	kinematic viscosity
α	$=$	$\frac{k}{\rho C_p}$	diffusivity
ρ			density
$\mathbf{g}$			gravitation
$\mathbf{g}\beta\Delta S$			bouiancy force

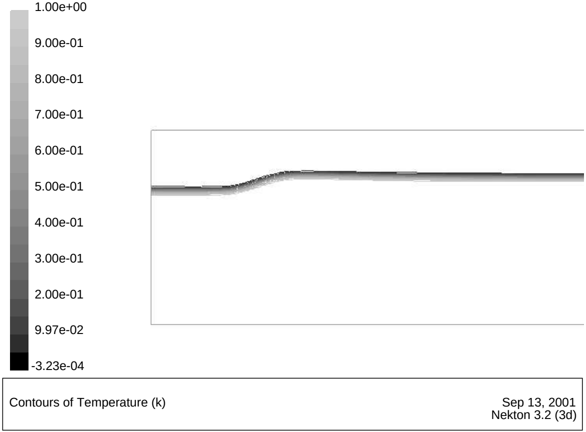
Simulation with spectral element method



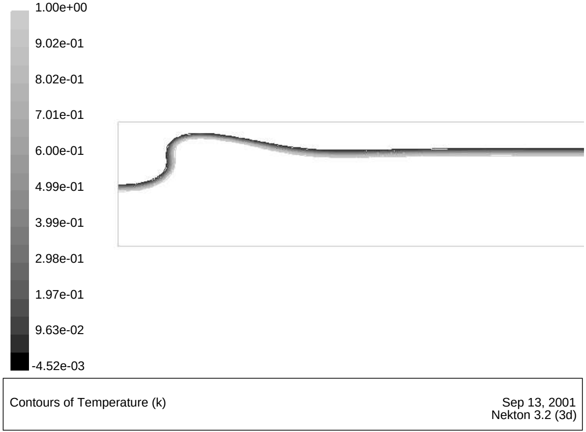
Simulation with spectral element method



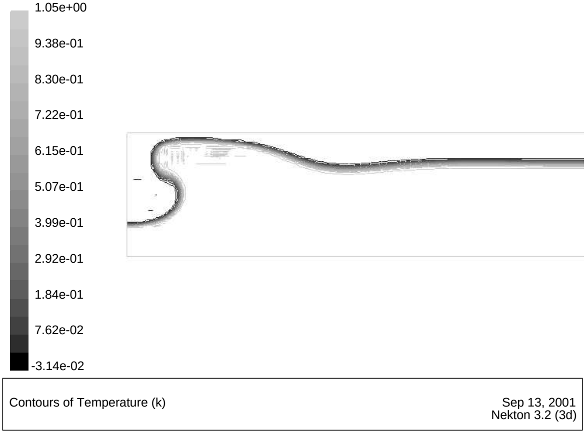
Simulation with spectral element method



Simulation with spectral element method



Simulation with spectral element method



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

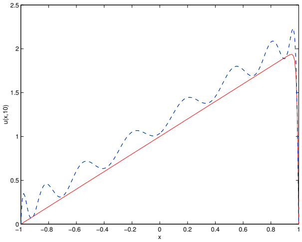
A linear convection diffusion problem in 1D

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

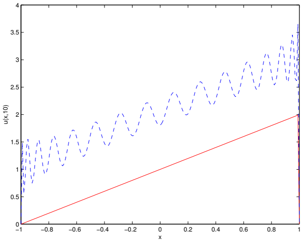
$u(x, 0) = \cos(x\pi/2)$ and homogeneous Dirichlet BCs.

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

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

A simple method

We consider a first order integrator for

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

Example

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

The exponential $\exp(hC(w)) \cdot g$ is the numerical approximation of the pure convection problem

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

$$\frac{Du}{Dt} := u_t + \mathbf{V} \cdot \nabla u.$$

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

$$\frac{D\tilde{u}_n}{Dt} = 0, \quad \tilde{u}_n(x, t_n) = u_n(x), \quad \text{on } [t_n, t_n + h]$$

$$\tilde{u}_n(x) := \tilde{u}_n(x, t_n + h)$$

$$u_{n+1} = \tilde{u}_n + h\nu\nabla^2 u_{n+1} + hf,$$

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

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

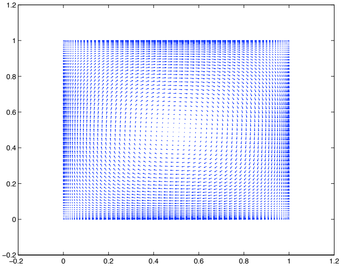
$$
\begin{aligned}
\frac{D\tilde{u}_n}{Dt} &= 0, \ \ \tilde{u}_n(x, t_n) = u_n(x), \ \ \text{on } [t_n, t_n + h] \\
&\qquad \tilde{u}_n(x) := \tilde{u}_n(x, t_n + h) \\
u_{n+1} &= \tilde{u}_n + h\nu\nabla^2 u_{n+1} + hf,
\end{aligned}
$$

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

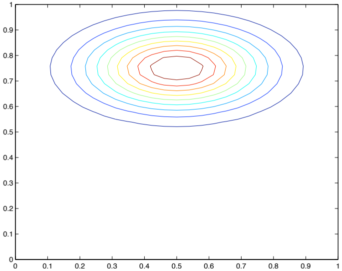
The exact integration of the pure convection problem can be obtained by introducing characteristics,

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

Linear convection: $\frac{Du}{Dt} = 0$.

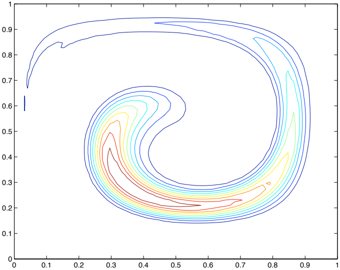


$$\mathbf{V} = \begin{bmatrix} \pi \sin(\pi x) \cos(\pi y) \\ -\pi \cos(\pi x) \sin(\pi y) \end{bmatrix}.$$

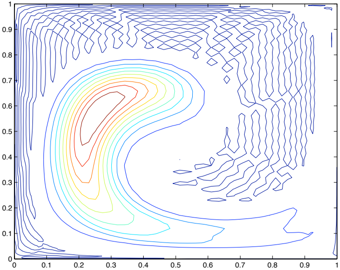


$$\mathbf{u}(x, y, 0) = e^{(-45(y-\frac{3}{4})^2 - 15(x-\frac{1}{2})^2)}$$

Linear convection: $\frac{Du}{Dt} = 0$

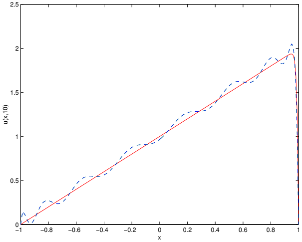


Characteristics in time + interpolation, $t = 1.2$.

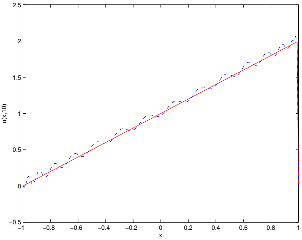


Semidiscretized convection + Krylov in time, $t = 1.2$.

Numerical tests with semi-Lagrangian spectral element methods: linear convection diffusion



$\nu = 0.01,\ K = 1,\ p = 16$



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

(Celledoni 2003)

The integration methods

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

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

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

$$\begin{array}{c|c} \mathbf{c} & A \\ \hline & \mathbf{b} \end{array} \qquad \begin{array}{c|c} \mathbf{c} & \hat{A} \\ \hline & \hat{\mathbf{b}} \end{array} \qquad \hat{a}_{i,j} := \sum_{l=1}^{J} \alpha_{il}^j, \quad \hat{b}_j := \sum_{l=1}^{J} \beta_l^j, \quad c_i = \hat{c}_i$$

Remarks

- The methods require the solution of only one (symmetric) linear system per stage.

Remarks

- The methods require the solution of only one (symmetric) linear system per stage.
- These methods can be viewed as partitioned Runge-Kutta /Commutator free methods for the transformed problem

$$y(t) = W(t)z(t), \quad \dot{W} = C(Wz)W, \quad \dot{z} = W^{-1}AWz.$$

Remarks

- The methods require the solution of only one (symmetric) linear system per stage.
- These methods can be viewed as partitioned Runge-Kutta /Commutator free methods for the transformed problem

$$y(t) = W(t)z(t), \quad \dot{W} = C(Wz)W, \quad \dot{z} = W^{-1}AWz.$$

Commutator-free method

for $r = 1 : s$ do

$$W_r = \exp(\textstyle\sum_k \alpha_{rJ}^k C_k) \cdots \exp(\sum_k \alpha_{r1}^k C_k)(p)$$

$$C_r = hC(W_r)$$

end

$W_1 = \exp(\sum_k \beta_J^k C_k) \cdots \exp(\sum_k \beta_1^k C_k)p$

Remarks

- The methods require the solution of only one (symmetric) linear system per stage.
- These methods can be viewed as partitioned Runge-Kutta /Commutator free methods for the transformed problem

$$y(t) = W(t)z(t), \quad \dot{W} = C(Wz)W, \quad \dot{z} = W^{-1}AWz.$$

Commutator-free method

for $r = 1 : s$ do

$$W_r = \exp(\sum_k \alpha_{rJ}^k C_k) \cdots \exp(\sum_k \alpha_{r1}^k C_k)(p)$$

$$C_r = hC(W_r)$$

end

$$W_1 = \exp(\sum_k \beta_J^k C_k) \cdots \exp(\sum_k \beta_1^k C_k) p$$

- Under reasonable simplifying assumptions the order condition up to order three coincide with the order conditions for Partitioned Runge-Kutta methods.

Order 2

Example

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

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

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.

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

Linear case

for $i = 1 : s$ do

$$Y_i = \exp(c_i hC) y_n + h \sum_{j=1}^{i} a_{i,j} \exp((c_i - c_j) hC) A Y_j$$

end

$$y_{n+1} = \exp(hC) y_n + h \sum_{i=1}^{s} b_i \exp((1 - c_i) hC) A Y_i$$

$$y_1 = (I - \frac{h}{2} A)^{-1} (I + \frac{h}{2} A) \exp(\frac{h}{2} C) y_0, \quad \text{order } 2.$$

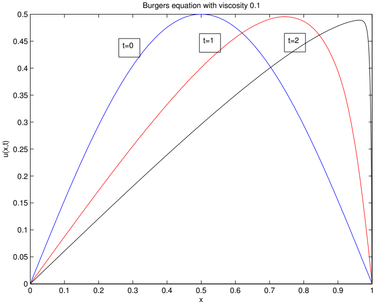
NUMERICAL TESTS

Viscous Burgers' equation

We consider

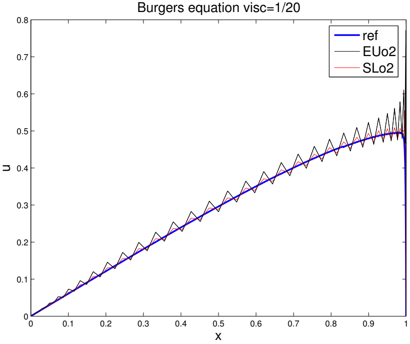
$$\frac{\partial}{\partial t}u + u\frac{\partial}{\partial x}u = \nu \nabla^2 u$$

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

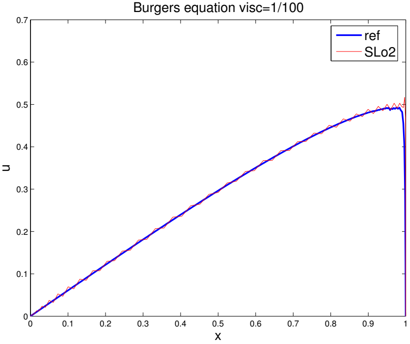


$$\nu = 1/10,\ K = 50,\ p = 8$$

Nonlinear test example



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



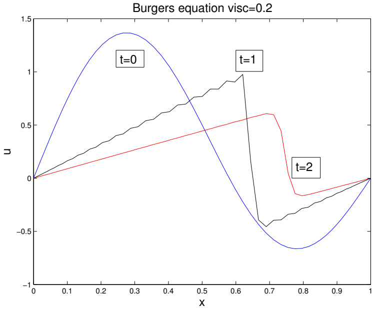
$\nu = 0.01,\ K = 1,\ p = 64$

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 and future work

- Seams that exponential integrators can be applied successfully in some convection dominated problems.
- Compute the exponential of the convection tracing particles (computing characteristics),gives an evident improvement compared to the "Eulerian" counterpart, but requires interpolation.
- Alternatively one could resolve more accurately the convection by increasing the number of grid points, integrating accurately a very well resolved convection problem, and projecting back the result on the original grid.
- This would require the availability of efficient methods for the approximation of the exponential of semidiscretized convection problems.

Thanks

Thanks. . .

for your attention!