1

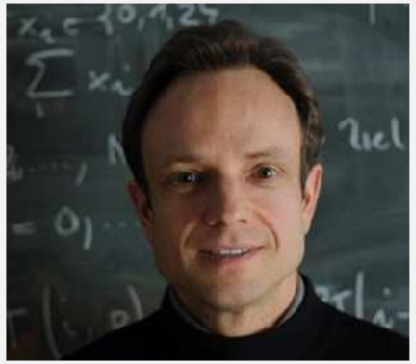
ETH Lecture 401-0674-00L Numerical Methods for Partial Differential Equations

Course Video
Section 10.3.3: Lagrangian Split-Step Method

Prof. R. Hiptmair, SAM, ETH Zurich

Date: May 3, 2022

(C) Seminar für Angewandte Mathematik, ETH Zürich



Dependencies. [Lecture → Section 7.5], [Lecture → Section 10.3.2]

Duration: 40 minutes

Note: Possible minor *mismatch of video and tablet notes*!

[Corrections and updates can be incorporated into tablet notes only]

X. Convection-Diffusion Problems

10.3. Discretization of Transient Convection-Diffusion IBVPs

10.3.3. Lagrangian Split-Step Method

→ based on method of characteristics ("particle tracking")

separate treatment of convection and diffusion

10.3.3.1. Split-Step Timestepping (→ Sect 7.5)

r.h.s = sum of two functions

$$\dot{\mathbf{y}} = \mathbf{g}(t,\mathbf{y}) + \mathbf{r}(t,\mathbf{y}) \;, \quad \mathbf{g},\mathbf{r} : [0,T] \times \mathbb{R}^m \mapsto \mathbb{R}^m \,. \qquad (10.3.3.1)$$

Idea: In turns solve

(1) $\dot{\mathbf{y}}(t) = \mathbf{g}(t,\mathbf{y})$,
(2) $\dot{\mathbf{y}}(t) = \mathbf{r}(t,\mathbf{y})$,

over small timesteps.

2

More details: [temporal mesh $0=t_0<t_1<t_2<\dots<t_M=T$]

Strang splitting single step method for (10.3.3.1), timestep $\tau := t_j - t_{j-1} > 0$:
compute $\mathbf{y}^{(j)} \approx \mathbf{y}(t_j)$ from $\mathbf{y}^{(j-1)} \approx \mathbf{y}(t_{j-1})$ according to

1. $\tilde{\mathbf{y}} := \mathbf{z}(t_{j-1}+\frac{1}{2}\tau)$, where $\mathbf{z}(t)$ solves $\dot{\mathbf{z}} = \mathbf{g}(t,\mathbf{z})$, $\mathbf{z}(t_{j-1}) = \mathbf{y}^{(j-1)}$, (10.3.3.2)
2. $\hat{\mathbf{y}} := \mathbf{w}(t_j)$, where $\mathbf{w}(t)$ solves $\dot{\mathbf{w}} = \mathbf{r}(t,\mathbf{w})$, $\mathbf{w}(t_{j-1}) = \tilde{\mathbf{y}}$, (10.3.3.3)
3. $\mathbf{y}^{(j)} := \mathbf{z}(t_j)$, where $\mathbf{z}(t)$ solves $\dot{\mathbf{z}} = \mathbf{g}(t,\mathbf{z})$, $\mathbf{z}(t_{j-1}+\frac{1}{2}\tau) = \hat{\mathbf{y}}$. (10.3.3.4)

↳ practise: by another SSM

Theorem 10.3.3.5. Order of Strang splitting single step method

Assuming exact solution of the initial value problems of the sub-steps, the Strang splitting single step method for (10.3.3.1) *is of second order.*

Apply to CDE:
$$\begin{array}{ccccccc} \frac{\partial u}{\partial t} & = & \epsilon\Delta u & + & f - \mathbf{v}\cdot\mathbf{grad}\,u \\ \updownarrow & & \updownarrow & & \updownarrow \\ \dot{\mathbf{y}} & = & \mathbf{g}(\mathbf{y}) & + & \mathbf{r}(\mathbf{y}) \end{array}$$

▷ Strang split-step method for convection-diffusion evolution eq.:
(w/ Dirichlet b.c. $u(x,t) = g(x,t)$, $(x,t)\in\partial\Omega\times]0,T[$)

1

(10.3.3.2) $\leftrightarrow$
$$\begin{aligned} &\frac{\partial w}{\partial t} - \epsilon\Delta w = 0 \quad \text{in } \Omega\times]t_{j-1}, t_{j-1}+\tfrac{1}{2}\tau[\,, \\ &w(\boldsymbol{x},t) = g(\boldsymbol{x},t) \quad \forall \boldsymbol{x}\in\partial\Omega,\ t_{j-1}<t<t_{j-1}+\tfrac{1}{2}\tau\,, \\ &w(\boldsymbol{x},t_{j-1}) = u^{(j-1)}(\boldsymbol{x}) \quad \forall \boldsymbol{x}\in\Omega\,. \end{aligned} \tag{10.3.3.6}$$

≙ parabolic IBVP

2

(10.3.3.3) $\leftrightarrow$
$$\begin{aligned} &\frac{\partial z}{\partial t} + \mathbf{v}(\boldsymbol{x},t)\cdot\mathbf{grad}\,z = f(\boldsymbol{x},t) \quad \text{in } \Omega\times]t_{j-1},t_j[\,, \\ &z(\boldsymbol{x},t) = g(\boldsymbol{x},t) \quad \text{on inflow boundary } \Gamma_{\text{in}},\ t_{j-1}<t<t_j\,, \\ &z(\boldsymbol{x},t_{j-1}) = w(\boldsymbol{x},t_{j-1}+\tfrac{1}{2}\tau) \quad \forall \boldsymbol{x}\in\Omega\,. \end{aligned} \tag{10.3.3.7}$$

≙ pure transport problem

3

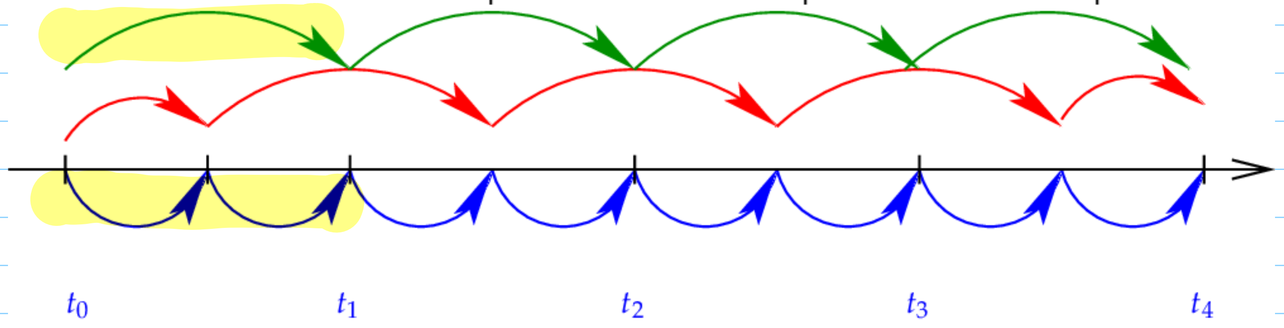
(10.3.3.4) $\leftrightarrow$
$$\begin{aligned} &\frac{\partial w}{\partial t} - \epsilon\Delta w = 0 \quad \text{in } \Omega\times]t_{j-1}+\tfrac{1}{2}\tau, t_j[\,, \\ &w(\boldsymbol{x},t) = g(\boldsymbol{x},t) \quad \forall \boldsymbol{x}\in\partial\Omega,\ t_{j-1}+\tfrac{1}{2}\tau<t<t_j\,, \\ &w(\boldsymbol{x},t_{j-1}+\tfrac{1}{2}\tau) = z(\boldsymbol{x},t_j) \quad \forall \boldsymbol{x}\in\Omega\,. \end{aligned} \tag{10.3.3.8}$$

Then set $u^{(j)}(\boldsymbol{x}) := w(\boldsymbol{x},t_j)$, $\boldsymbol{x}\in\Omega$.

≙ parabolic IBVP

Rem 10.3.3.9: (Leap-Frog implementation of Strang splitting)

combine the last sub-step ③ with the first sub-step ① of the next timestep



—: sub-step ②, —: sub-step ① & ③

10.3.3.2 Particle Method for Pure Transport

Recall MOC solution ($\to$ Sect 10.3.2)

$$\frac{\partial u}{\partial t} + \mathbf{v}(\boldsymbol{x},t)\cdot \mathbf{grad}\, u = f \quad \text{in } \tilde{\Omega} := \Omega\times]0,T[\,,$$
$$u(\boldsymbol{x},t) = g(\boldsymbol{x},t) \quad \text{on} \quad \Gamma_{\text{in}}\times]0,T[\quad,\quad u(\boldsymbol{x},0) = u_0(\boldsymbol{x}) \quad \text{in } \Omega\,, \tag{10.3.3.11}$$

$$\Gamma_{\text{in}} := \{\boldsymbol{x}\in\partial\Omega\colon \mathbf{v}(\boldsymbol{x})\cdot\boldsymbol{n}(\boldsymbol{x}) < 0\}\,. \tag{10.2.1.11}$$

Case $f\equiv 0$:

$$\blacktriangleright \quad u(\boldsymbol{x},t) = \begin{cases} u_0(\boldsymbol{x}_0) & \text{, if } \boldsymbol{y}(s)\in\Omega \quad \forall 0<s<t\,, \\ g(\mathbf{y}(s_0),s_0) & \text{, if } \boldsymbol{y}(s_0)\in\partial\Omega, \boldsymbol{y}(s)\in\Omega \quad \forall s_0<s<t\,, \end{cases} \tag{10.3.3.12}$$

for $(\boldsymbol{x},t)\in\tilde{\Omega}$, where $s\mapsto\mathbf{y}(s)$ solves the initial value problem for the streamline ODE

$$\frac{d\mathbf{y}}{ds}(s) = \mathbf{v}(\mathbf{y}(s),s) \quad,\quad \mathbf{y}(t) = \boldsymbol{x}\,, \tag{10.3.3.13}$$

fluid particle trajectory

general f:

$$\blacktriangleright \quad u(\boldsymbol{x},t) = \begin{cases} u_0(\boldsymbol{x}_0) + \int_0^t f(\mathbf{y}(s),s)\,\mathrm{d}s & \text{, if } \boldsymbol{y}(s)\in\Omega \quad \forall 0<s<t\,, \\ g(\mathbf{y}(s_0),s_0) + \int_{s_0}^t f(\mathbf{y}(s),s)\,\mathrm{d}s & \text{, if } \boldsymbol{y}(s_0)\in\partial\Omega, \boldsymbol{y}(s)\in\Omega \quad \forall s_0<s<t\,. \end{cases}$$

(10.3.2.7)

Particle method = forward tracking of particles

I. Pick initial particle locations $p_i\in\Omega$, $i=1,\dots,N$

II. "Particle pushing": Apply SSM to IVPs

$$\dot{y}(t) = v(y(t),t)\,,\quad y(0) = p_i\,,$$

timestep $\tau := T/M$

$\triangleright$ sequence $\left(p_i^{(j)} := y^{(j)}\right)_{j=0}^{M}$, $i=1,\dots,N$

III. Reconstruct approximation $u_h^{(j)} \approx u(\cdot, t_j := j\tau)$ by interpolation:

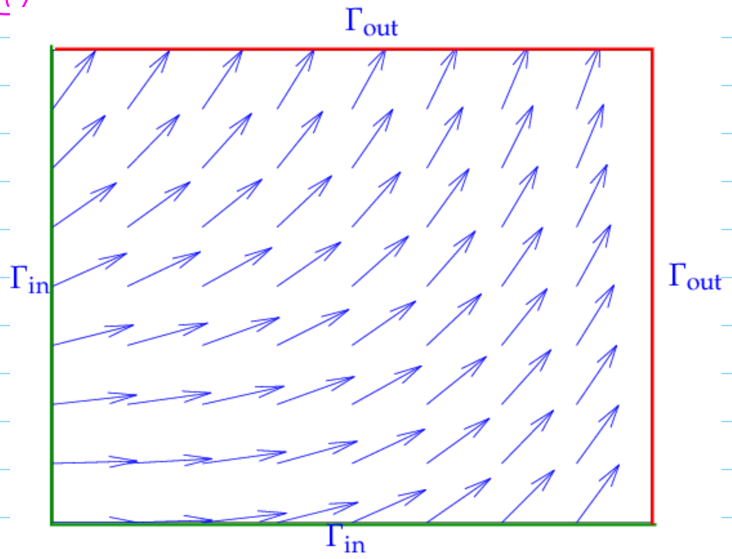
MOC formula

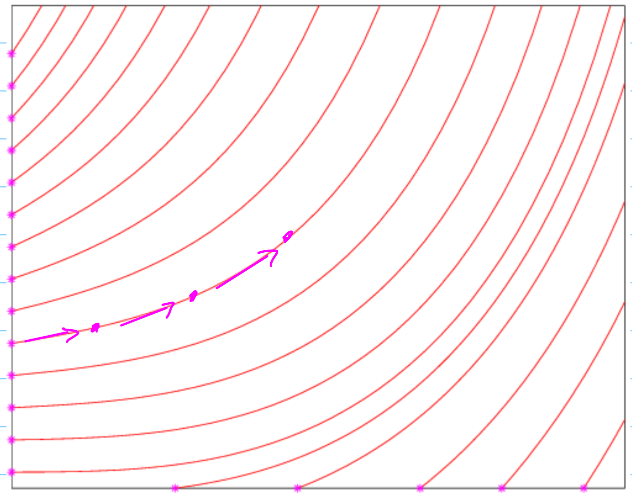
$$u_h^{(j)}(\boldsymbol{p}_i^{(j)}) := u_0(\boldsymbol{p}_i) + \tau\sum_{l=1}^{j-1} f\left(\tfrac{1}{2}(\boldsymbol{p}_i^{(l)} + \boldsymbol{p}_i^{(l-1)}), \tfrac{1}{2}(t_l + t_{l-1})\right),\quad i=1,\dots,N\,.$$

for no in/outflow: $v\cdot n = 0$ on $\partial\Omega$

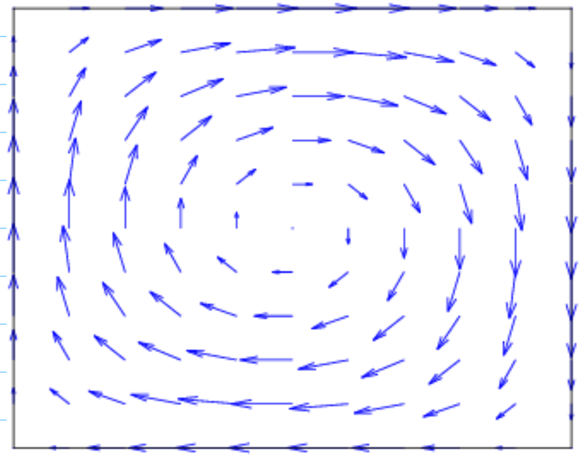
Remark 10.3.3.15 (Particle method adapted to in/outflow)

- Drop particles leaving Ω in Step II
- "Inject" particles at Γ_{in}

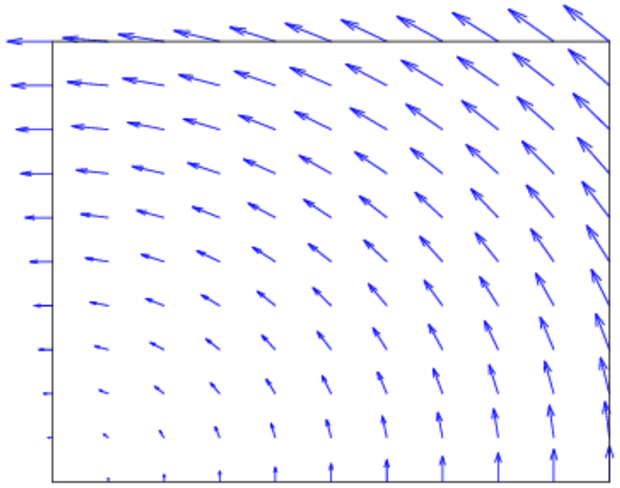




$\bullet \triangleq$ injected particles



velocity field $\mathbf{v}_1$ (`circvel`)



velocity field $\mathbf{v}_2$ (`rotvel`)

Exp. 10.3.3.16 (Point particle method for pure advection)

- IBVP (10.3.3.11) on $\Omega =]0,1[^2$, $T = 2$, with $f \equiv 0$, $g \equiv 0$.
- Initial locally supported bump $u_0(\boldsymbol{x}) = \max\{0, 1 - 4\left\|\boldsymbol{x} - \begin{bmatrix} 1/2 \\ 1/4 \end{bmatrix}\right\|\}$.
- Two stationary divergence-free velocity fields
  - $\mathbf{v}_1(\boldsymbol{x}) = \begin{bmatrix} -\sin(\pi x_1)\cos(\pi x_2) \\ \cos(\pi x_1)\sin(\pi x_2) \end{bmatrix}$ satisfying (10.1.1.5),
  - $\mathbf{v}_2(\boldsymbol{x}) = \begin{bmatrix} -x_2 \\ x_1 \end{bmatrix}$.
- Initial positions of interpolation points on regular tensor product grid with meshwidth $h = \frac{1}{40}$.
- Approximation of trajectories by means of explicit trapezoidal rule (method of Heun).

$\triangleright$ Animation

No artificial diffusion : no smearing/damping

10.3.3.3 Particle Mesh Method (PPM)

Strang split-step method:

In turns solve
→ Pure transport IBVP : Particle method
→ Parabolic IBVP : MOL

How to combine both?

Idea: two views

"particle temperatures" $u(\boldsymbol{p}_i^{(j)})$

$\updownarrow$

Nodal values of finite element function $u_h^{(j)} \in \mathcal{S}_1^0(\mathcal{M})$

Discussion for CD-IBVP

$$\begin{cases} \dfrac{\partial u}{\partial t} - \epsilon\Delta u + \mathbf{v}(\boldsymbol{x})\cdot\mathbf{grad}\,u = f \quad \text{in } \widetilde{\Omega} := \Omega\times]0,T[\,, \\ u(\boldsymbol{x},t) = 0 \quad \forall \boldsymbol{x}\in\partial\Omega, 0<t<T \quad , \quad u(\boldsymbol{x},0) = u_0(\boldsymbol{x}) \quad \forall\boldsymbol{x}\in\Omega\,. \end{cases} \tag{10.3.1.1}$$

→ Single timestep of PPM of size $\tau > 0$: $t_{j-1} \longrightarrow t_j$

given : • mesh $\mathcal{M}^{(j-1)}$

• $u_h^{(j-1)} \in \mathcal{S}_{1,0}^0(\mathcal{M}^{(j-1)})$

I. Diffusion (half) step :

$\{\mathcal{S}_{1,0}^0(\mathcal{M}_{j-1})$-FE + implicit RK-SSM$\}$ - MOL for

$$\frac{\partial w}{\partial t} - \epsilon\Delta w = 0 \quad \text{in } \Omega\times]t_{j-1}, t_{j-1}+\tfrac{1}{2}\tau[\,,$$
$$w(\boldsymbol{x},t) = 0 \quad \forall\boldsymbol{x}\in\partial\Omega,\ t_{j-1} < t < t_{j-1}+\tfrac{1}{2}\tau\,,$$
$$w(\boldsymbol{x},t_{j-1}) = u_h^{(j-1)}(\boldsymbol{x}) \quad \forall\boldsymbol{x}\in\Omega\,.$$

II. Advection step :

Particle method for pure transport IBVP

$$\frac{\partial z}{\partial t} + \mathbf{v}(\boldsymbol{x},t)\cdot\mathbf{grad}\,z = f(\boldsymbol{x},t) \quad \text{in } \Omega\times]t_{j-1},t_j[\,,$$
$$z(\boldsymbol{x},t) = 0 \quad \text{on inflow boundary } \Gamma_{\text{in}},\ t_{j-1}<t<t_j\,,$$
$$z(\boldsymbol{x},t_{j-1}) = w_h(\boldsymbol{x},t_{j-1}+\tfrac{1}{2}\tau) \quad \forall\boldsymbol{x}\in\Omega\,.$$

• Initial particle locations $p_i \in \Omega$ = nodes of $\mathcal{M}^{(j-1)}$

• $z(p_i) = w_h(p_i, t_{j-1} + \tfrac{1}{2}\tau)$

III. Remeshing:

$\mathcal{M}^{(f)}$ = mesh with nodes ≙ final particle locations

IV. Diffusion (half) step on $\mathcal{M}^{(f)}$

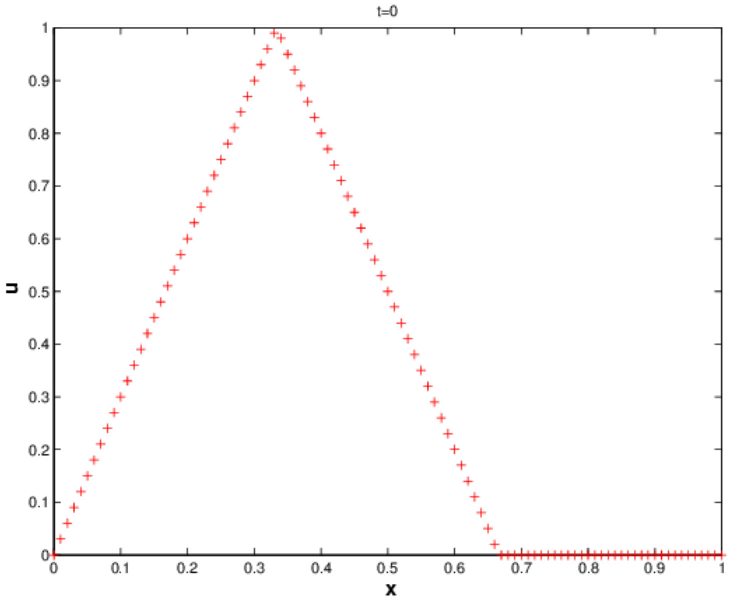
Exp. 10.3.3.20 (PPM for 1D CD-IBVP)

Same IBVP (10.3.1.4) as in Exp. 10.3.1.3:

$$\frac{\partial u}{\partial t} - \epsilon\frac{\partial^2 u}{\partial x^2} + \frac{\partial u}{\partial x} = 0\,,$$
$$u(x,0) = \max(1 - 3|x - \tfrac{1}{3}|, 0)\,,$$
$$u(0) = u(1) = 0\,.$$

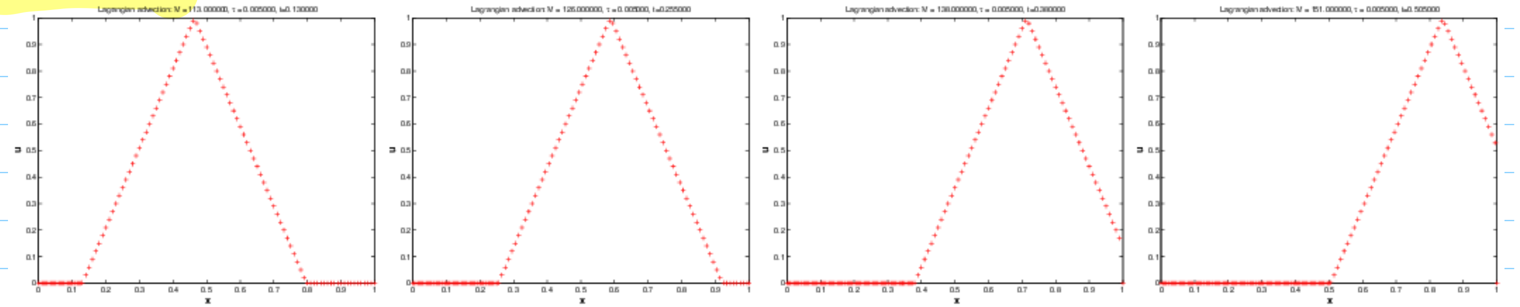
- Linear finite element Galerkin discretization with mass lumping in space
- Strang splitting applied to diffusive and convective terms
- (Sub-optimal) implicit Euler timestepping for diffusive partial timestep

$x \mapsto u_0(x)$ ▷



Convection-dominated:

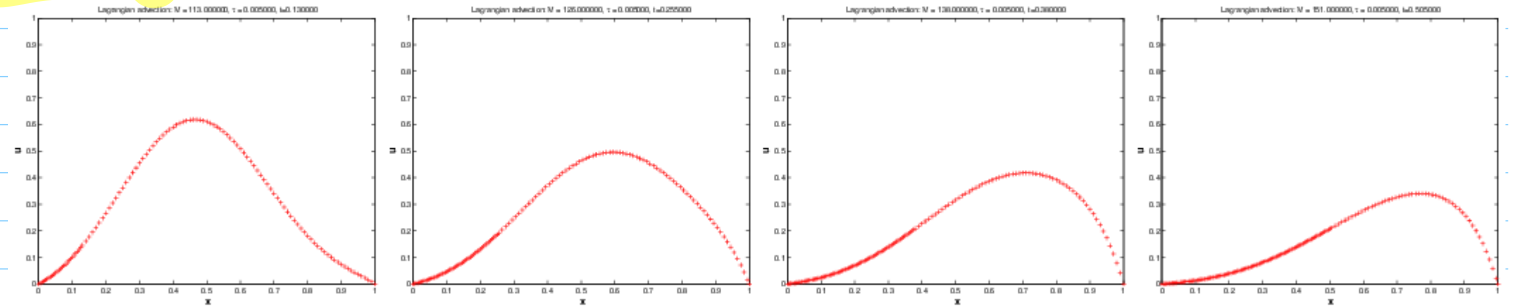
$\epsilon = 10^{-5}$:



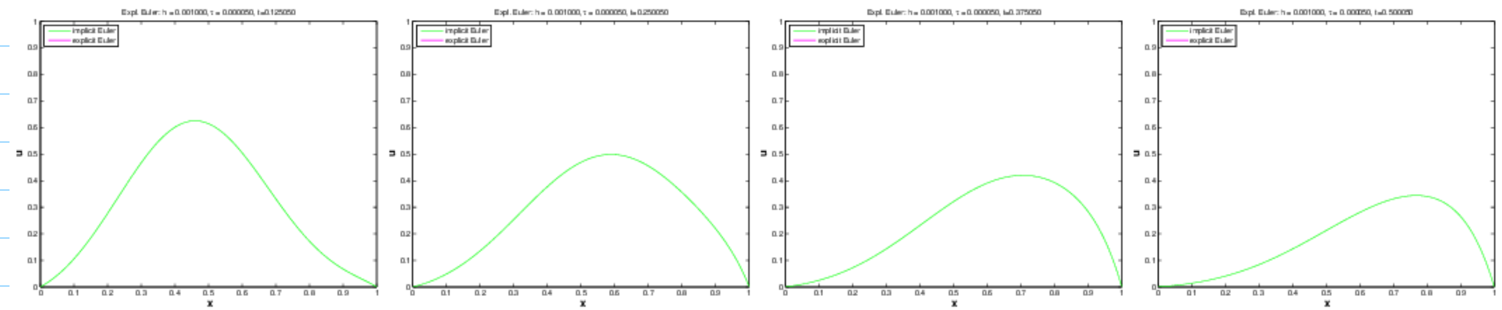
→ No spurious diffusion

Significant diffusion

$\epsilon = 0.1$:

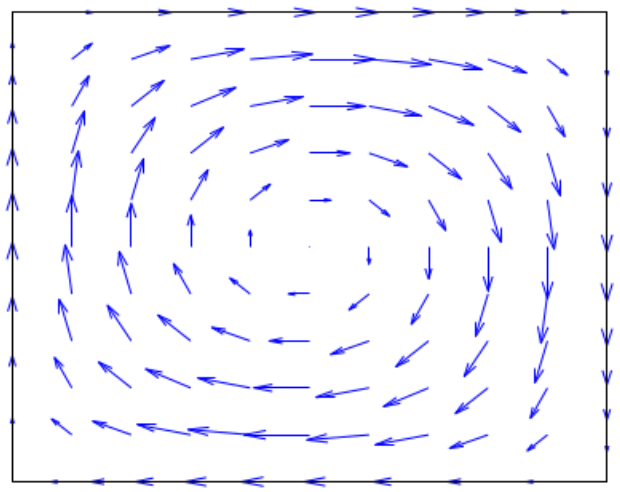


“Reference solution” computed by method of lines, see Exp. 10.3.1.3, with $h = 10^{-3}$, $\tau = 5\cdot 10^{-5}$ (“overkill resolution”):



→ Good agreement

Exp 10.3.3.21 (PMM for CD-IVP in 2D)



$\varepsilon = 10^{-3}$

$\Omega =]0,1[^2$

$\triangleleft$ velocity field $\underline{v}$

Delaunay remeshing
[qhull library]

$\triangleright$ Animation

Summary:

Advantage of Lagrangian (particle) methods for convection diffusion:

- No artificial diffusion required (no "smearing")

  No stability induced timestep constraint

Drawback of Lagrangian (particle) methods for convection diffusion:

- Remeshing (may be) expensive and difficult.

  Point advection may produce "voids" in point set.

$\triangleright$ Review questions 10.3.3.22