A second order semi-Lagrangian discretization of the advection-diffusion-reaction equation

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22nd February 2023

Introduction

Motivations

- Systems of advection-diffusion-reaction equations are responsible for most of the computational cost of many models ;
- the choice of a method that allows the use of large time steps is of fundamental importance ;
- standard ways to achieve optimal efficiency : the use of implicit schemes or semi-Lagrangian techniques for the advection step, coupled to implicit methods for the diffusion and reaction step ;
- a fully semi-Lagrangian scheme is more efficient than standard implicit techniques ;
- in our work, we show how to obtain second order accuracy in time ;
- we propose a treatment of Dirichlet boundary conditions.

Semi-Lagrangian method for advection-diffusion-reaction
The equation

$$\begin{cases} c_t + u \cdot \nabla c - \nu \Delta c = f(c) & (x,t) \in \Omega \times (0,T], \\ c(x,t) = b(x,t) & (x,t) \in \partial\Omega \times (0,T], \\ c(x,0) = c_0(x) & x \in \Omega, \end{cases} \tag{1}$$

where :

- $\Omega \subset \mathbb{R}^2$ is a bounded open set ;
- $c : \Omega \times [0,T] \to \mathbb{R}$ can be interpreted as the concentration of a chemical species ;
- $u : \Omega \times [0,T] \to \mathbb{R}^2$ is a velocity field ;
- $f(c)$ is a source term responsible for a nonlinear evolution of c ;
- $b : \partial\Omega \times [0,T] \to \mathbb{R}$ denotes the boundary value of the species c.

Semi-Lagrangian method for advection-diffusion-reaction

The representation formula

Feynman-Kac formula :

$$c(x,t) = \mathbb{E}\left[c_0\left(y\left(x,t;0\right)\right) + \int_0^t f\left(c\left(y\left(x,t;s\right),s\right)\right)\mathrm{d}s\right], \tag{2}$$

where y solves

$$\begin{cases} \mathrm{d}y\left(x,t;s\right) = -u\left(y\left(x,t;s\right)\right)\mathrm{d}s + \sqrt{2\nu}\,\mathrm{d}W \\ y\left(x,t;t\right) = x. \end{cases} \tag{3}$$

In (3) :

- W is a Brownian motion starting at 0;
- $\mathrm{d}W$ indicates the limit for $\Delta t \to 0$ of the increments $\Delta W = W_{t+\Delta t} - W_t$.

Semi-Lagrangian method for advection-diffusion-reaction

Disctretization of the stochastic characteristics

To obtain a second order semi-discrete method in time :

- the interval $[0, T]$ must be discretized with a step $\Delta t > 0$: we denote $t^k = k\Delta t$, $k = 0, \dots, \lceil T/\Delta t \rceil$;
- the solution of (3) must be approximated with a second order method, such as stochastic Crank-Nicolson (implicit)

$$y_{k+1}(x) = y_k(x) - \frac{\Delta t}{2}\left(u\left(y_k, t^k\right) + u\left(y_{k+1}, t^{k+1}\right)\right) + \sqrt{6\nu\Delta t}\Delta W_k,$$

or stochastic Heun (explicit) :

$$y_{k+1}(x) = y_k(x) - \frac{\Delta t}{2}\left(u\left(y_k, t^k\right) + u\left(\overline{y}_{k+1}, t^{k+1}\right)\right) + \sqrt{6\nu\Delta t}\Delta W_k,$$

with $\overline{y}_{k+1}$ first order approximation of y_{k+1}.

Semi-Lagrangian method for advection-diffusion-reaction

Disctretization of the stochastic characteristics

- ΔW_k is discretized using the following vectors :

$$e_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad e_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad e_3 = \begin{pmatrix} 0 \\ -1 \end{pmatrix},$$
$$e_4 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad e_5 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \quad e_6 = \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$
$$e_7 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad e_8 = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \quad e_9 = \begin{pmatrix} -1 \\ -1 \end{pmatrix},$$

- the distribution of the discretization of ΔW_k is given by :

$$\alpha_1 = 4/9, \alpha_2 = \alpha_3 = \alpha_4 = \alpha_5 = 1/9, \alpha_6 = \alpha_7 = \alpha_8 = \alpha_9 = 1/36.$$

Semi-Lagrangian method for advection-diffusion-reaction

Semi-discrete method and fully discrete method

The semi-discrete scheme in time is :

$$c^{n+1}(x) = \sum_{k=1}^{9} \alpha_k \left(c^n \left(y^{n+1}(x) \right) + \frac{\Delta t}{2} f \left(c^n \left(y^{n+1}(x) \right) \right) \right) + \frac{\Delta t}{2} f \left(c^{n+1}(x) \right).$$

- Given $\Delta x > 0$, we get a triangulation $\mathcal{G}_{\Delta x} = \left\{ x_i : x_i \in \overline{\Omega} \right\}$;
- an interpolation operator of degree p, $I_p[\cdot]$, must be chosen.

$$c_i^{n+1} = \sum_{k=1}^{9} \alpha_k \left(I_p[c^n] \left(y_i^{n+1} \right) + \frac{\Delta t}{2} f \left(I_p[c^n] \left(y_i^{n+1} \right) \right) \right) + \frac{\Delta t}{2} f \left(c_i^{n+1} \right).$$

Convergence analysis

For simplicity, we studied the convergence of the scheme for :

- a one-dimensional problem ;
- without boundary, i.e. $\Omega = \mathbb{R}$;
- with a time-independent advection term u.

We'll use the following notation :

$$c_i^{n+1} = S_{\Delta t, \Delta x}\left(c^{n+1}, c^n, x_i\right), \text{ for } i \in \mathbb{Z} \text{ and } n = 0, \dots, N-1, \quad (4)$$

$$y_\pm(x) = x - \frac{\Delta t}{2}\left[u(x) + u(y_\pm(x))\right] \pm \sqrt{6 \Delta t \nu}, \quad (5)$$

$$y_0(x) = x - \frac{\Delta t}{2}\left[u(x) + u(y_0(x))\right], \quad (6)$$

with $\alpha_\pm = 1/6$ e $\alpha_0 = 2/3$.

Convergence analysis

Consistency

Proposition

Assume $u \in C^2(\mathbb{R})$ *e* $f \in C^4(\mathbb{R})$, *and that there exist two constants* K_1 *and* K_2, *independent from* x *and* t, *such that* $|f^{(m)}(x)| \leq K_1$ *for* $m \leq 4$ *and* $|u^{(m)}(x)| \leq K_2$ *for* $m \leq 2$ *; let* $c(x,t)$ *be a classical solution of* (1). *Then, for all* $(i,n) \in \mathbb{Z} \times \{0, \ldots, N-1\}$ *the consistency error of the scheme*

$$\mathcal{T}_{\Delta t, \Delta x}(x_i, t^n) = \frac{1}{\Delta t}\left(c\left(x_i, t^{n+1}\right) - S_{\Delta t, \Delta x}\left(c\left(t^n\right), c\left(t^{n+1}\right), x_i, t^n\right)\right),$$

where $c(t_n) = (c(x_i, t^n))_i$, *is such that*

$$\mathcal{T}_{\Delta t, \Delta x}(x, t) = \mathcal{O}\left(\Delta t^2 + \frac{\Delta x^p}{\Delta t}\right).$$

Convergence analysis

Stability

To prove stability we write the method in matrix form :

$$c^{n+1} - \frac{\Delta t}{2} f\left(c^{n+1}\right) = \sum_k \alpha_k \left[B_k c^n + \frac{\Delta t}{2} f\left(B_k c^n\right) \right],$$

where $b_{k,ij} = \psi_j\left(y_k\left(x_i\right)\right)$, with ψ_j basis function.

Proposition

Assume $f(x) \in C^4(\mathbb{R})$, and that there exists a constant K independent from x and t such that $|f^{(m)}(x)| \leq K$ for $m \leq 4$. Then, for each k, there exists a constant $C_B > 0$ independent from Δx and Δt such that

$$\|B_k\| \leq 1 + C_B \Delta t.$$

Convergence analysis

Convergence

Theorem

Assume the existence of a classical solution of (1)*, that* $f(x) \in C^4(\mathbb{R})$ *and* $u(x) \in C^2(\mathbb{R})$*, and that there exist two constants* K_1 *e* K_2*, independent from* x *and* t*, such that* $|f^{(m)}(x)| \leq K_1$ *for* $m \leq 4$ *and* $|u^{(m)}(x)| \leq K_2$ *for* $m \leq 2$*. Let* $c(x,t)$ *be the classical solution of* (1) *and* (c_i^n) *the solution of* (4)*. Then, for all* n *such that* $t^n \in [0,T]$*, as* $(\Delta t, \Delta x) \to 0$*,*

$$\|c(t_n) - c^n\|_2 \leq C\left(\Delta t^2 + \frac{\Delta x^p}{\Delta t}\right),$$

where C *is a positive constant depending on* T*.*

Dirichlet boundary conditions

Existing methods for treating Dirichlet boundary conditions are :

- of first order and not generalizable to multi-dimensional problems ;
- of order one half, adaptable to all space dimensions.

Our method consists in constructing two meshes :

- the first given by $\mathcal{G}_{\Delta x} = \left\{ x_i, x_i \in \overline{\Omega} \right\}$;
- given an $h > 0$, we consider a second mesh, $\mathcal{G}_h = \left\{ v_i, v_i \in \overline{\Omega} \right\}$, only built around the boundary and made up of triangular or rectangular elements. On each of those elements we consider the following degrees of freedom : the vertices, the midpoints of the edges and the the center of mass.

Dirichlet boundary conditions

Then, for each $(v_i) \in \mathcal{G}_h$:

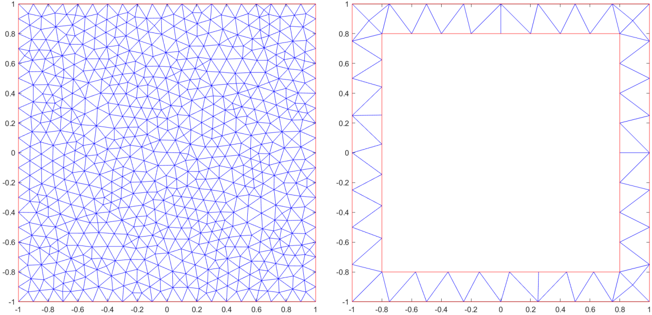
- if the point is inside the domain, then the solution is obtained by interpolation ;
- if the point is on the boundary $\partial\Omega$, then we set the Dirichlet condition on that point.

If, for some k and some i, one of the characteristics falls outside the domain ($y_i^k \notin \overline{\Omega}$), then :

- we compute its projection $\mathcal{P}\left(y_i^k\right)$ on $\overline{\Omega}$;
- the numerical solution on $\mathcal{P}\left(y_i^k\right)$ is approximated by a quadratic polynomial, built using basis $\mathbb{P}_2$ or $\mathbb{Q}_2$ associated to $\mathcal{G}_h$.

Dirichlet boundary conditions

Figure – Example of grids $\mathcal{G}_{\Delta x}$ and $\mathcal{G}_h$ on a squared domain



(a) $\mathcal{G}_{\Delta x}$ (b) $\mathcal{G}_h$

Dirichlet boundary conditions

Analysis

- Let $h > \max_i \left| y_i^k - x_i \right|$.
- h is of order $O(\Delta t^{1/2})$ for $\nu > 0$, it is of order $O(\Delta t)$ if $\nu = 0$.
- Let the extrapolation be performed with $N_{ex} + 1$ evenly spaced nodes ξ_k with step h. Then there exists a certain $C > 0$ such that for characteristics falling in this strip of width C outside of Ω the scheme remains stable.
- It is possible to prove that with our proposed treatment of the boundary conditions the truncation error becomes

$$\mathcal{T}_{\Delta t, \Delta x}(x,t) = \mathcal{O}\left(h^{N_{ex}+1} \Delta t^2 + \frac{\Delta x^p}{\Delta t} \right).$$

Numerical tests

We tried our method on different simulations :

- advection-diffusion equation with constant velocity field and non-homogeneous Dirichlet boundary conditions ;
- advection-diffusion equation with rotating velocity field and non-homogeneous Dirichlet boundary conditions ;
- Allen-Cahn equation with periodic boundary conditions ;
- advection-diffusion equation with non-homogeneous Dirichlet boundary conditions on a non-convex domain.

Numerical tests

Constant advection

The problem setting is :

- the domain is $\Omega = (-1,1) \times (-1,1)$;
- the velocity field is $u = (1,0)$;
- the diffusion coefficient is $\nu = 5 \cdot 10^{-2}$;
- the initial datum is a gaussian distribution centered in $(x_0, y_0) = (0.5, 0)$ with standard deviation $\sigma = 0.1$;
- the boundary condition is given by the exact solution of the problem :

$$c\,(x,y,t) = \frac{10 \exp\left\{ \frac{(x-x_0-t)^2+(y-y_0)^2}{2\left(\sigma^2+2\nu t\right)} \right\}}{1+2\nu/\sigma^2} \tag{7}$$

Numerical tests

Constant advection - errors

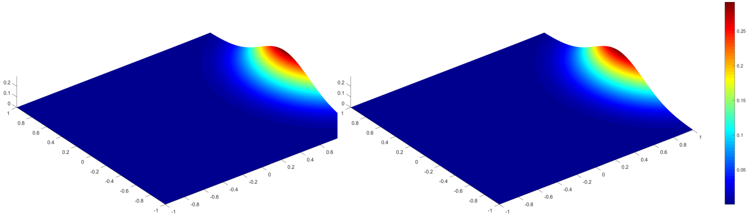
In the table $C = \frac{\Delta t \max |u|}{\Delta x}$. The value of $\mu = \frac{\Delta t \nu}{\Delta x^2}$ is greater than 0.5 in every simulation.

Δx_{max}	Δx_{min}	Δt	C_{min}	C_{max}	h	l_2	p_2
0.04	0.015	0.1	2.50	6.67	0.50	$7.79 \cdot 10^{-3}$	-
0.02	0.0075	0.05	2.50	6.67	0.17	$6.57 \cdot 10^{-4}$	3.58
Δx_{max}	Δx_{min}	Δt	C_{min}	C_{max}	h	l_2	p_2
0.04	0.015	0.05	1.25	3.33	0.50	$7.35 \cdot 10^{-3}$	-
0.02	0.0075	0.025	1.25	3.33	0.17	$3.76 \cdot 10^{-4}$	4.29
Δx_{max}	Δx_{min}	Δt	C_{min}	C_{max}	h	l_2	p_2
0.04	0.015	0.025	0.625	1.67	0.50	$8.35 \cdot 10^{-3}$	-
0.02	0.0075	0.0125	0.625	1.67	0.17	$2.64 \cdot 10^{-4}$	4.98

Numerical tests

Constant advection - plot

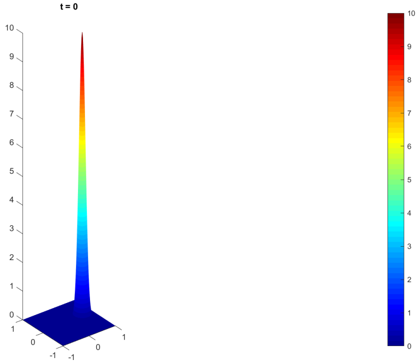
Figure – Comparison between numerical solution and exact solution



(a) Numerical solution (b) Exact solution

Numerical tests

Constant advection - video



Numerical tests

Rotating velocity field

The problem setting is :

- the domain is $\Omega = (-1, 1) \times (-1, 1)$;
- the velocity field is $u = (-2\pi y, 2\pi x)$;
- the diffusion coefficient is $\nu = 5 \cdot 10^{-2}$;
- the initial datum is a gaussian distribution centered in $(x_0, y_0) = (0.5, 0)$ with standard deviation $\sigma = 0.1$;
- the boundary condition is given by the exact solution of the problem :

$$c\,(x, y, t) = \frac{10 \exp \left\{ \frac{(x - x(t))^2 + (y - y(t))^2}{2\left(\sigma^2 + 2\nu t\right)} \right\}}{1 + 2\nu/\sigma^2} \tag{8}$$

with $x\,(t) = x_0 \cos 2\pi t - y_0 \sin 2\pi t$ and $y\,(t) = x_0 \sin 2\pi t - y_0 \cos 2\pi t$.

Numerical tests

Rotating velocity field - errors

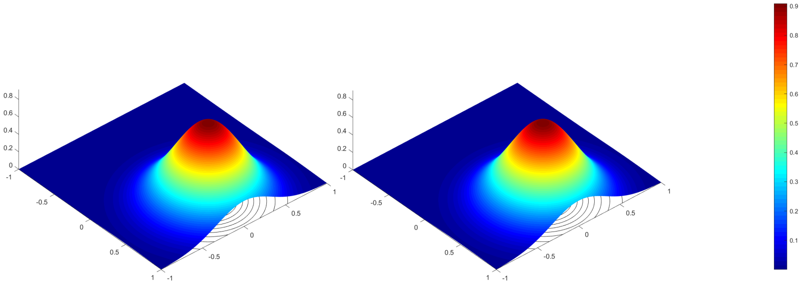
In the table $C = \frac{\Delta t \max |u|}{\Delta x}$. The value of $\mu = \frac{\Delta t \nu}{\Delta x^2}$ is greater than 0.5 in every simulation.

Δx_{max}	Δx_{min}	Δt	C_{min}	C_{max}	h	l_2	p_2
0.04	0.015	0.05	7.85	20.94	0.50	$5.62 \cdot 10^{-2}$	-
0.02	0.0075	0.025	7.85	20.94	0.17	$1.49 \cdot 10^{-2}$	1.91
Δx_{max}	Δx_{min}	Δt	C_{min}	C_{max}	h	l_2	p_2
0.04	0.015	0.025	3.92	10.47	0.50	$1.49 \cdot 10^{-2}$	-
0.02	0.0075	0.0125	3.92	10.47	0.17	$3.43 \cdot 10^{-3}$	2.12

Numerical tests

Rotating velocity field - plot

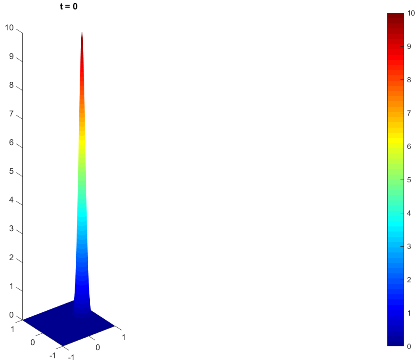
Figure – Comparison between numerical solution and exact solution



(a) Numerical solution (b) Exact solution

Numerical tests

Rotating velocity field - video



Numerical tests

Allen-Cahn equation

For the test on the Allen-Cahn equation we have the following data :

- the domain is $\Omega = (0,1) \times (0,1)$;
- the velocity field is constantly zero and there is a reaction term :

$$c_t = \nu \Delta c - c^3 + c; \tag{9}$$

- we used diffusion coefficients $\nu = 5 \cdot 10^{-2}$ and $\nu = 10^{-2}$;
- the initial datum is :

$$c_0\left(x, y\right) = \sin\left(2\pi x\right) \sin\left(2\pi y\right); \tag{10}$$

- periodic boundary conditions.

Numerical tests

Allen-Cahn equation - errors

- There is no exact solution for this problem : we computed the errors using a reference solution computed by a pseudo-spectral Fourier discretization in space and a fourth order Runge-Kutta scheme in time ;
- in this problem there is no velocity field : this means that there also is no Courant number. In the tables, we report the value of $\mu = \frac{\Delta t \nu}{\Delta x^2}$

Numerical tests

Allen-Cahn equation - errors

Δx	Δt	μ	l_2	l_∞	p_2	p_∞
0.04	0.1	0.62	$2.82 \cdot 10^{-2}$	$4.01 \cdot 10^{-2}$	-	-
0.02	0.05	1.25	$7.13 \cdot 10^{-3}$	$8.47 \cdot 10^{-3}$	1.98	2.24
0.01	0.025	2.5	$1.97 \cdot 10^{-3}$	$2.20 \cdot 10^{-3}$	1.86	1.94

Table – $\nu = 0.05$

Δx	Δt	μ	l_2	l_∞	p_2	p_∞
0.04	0.1	0.62	$1.10 \cdot 10^{-3}$	$1.31 \cdot 10^{-3}$	-	-
0.02	0.05	1.25	$2.72 \cdot 10^{-4}$	$2.98 \cdot 10^{-4}$	2.02	2.14
0.01	0.025	2.5	$6.53 \cdot 10^{-5}$	$7.06 \cdot 10^{-5}$	2.06	2.08

Table – $\nu = 0.01$

Numerical tests

Non-convex domain

- The domain is $\Omega = [0,1] \times [0,0.4] \setminus B_{r_0}(x_0, y_0)$, with $r_0 = 0.05$ and $(x_0, y_0) = (0.1, 0.2)$;
- the velocity field is

$$u(x,y) = \left(u_0 + \frac{u_0 r_0^3}{2r^3} - \frac{3u_0 r_0^3 (x - x0)^2}{2r^5}, -\frac{3r_0^3 u_0 (x - x0)(y - y0)}{2r^5} \right),$$

in which $u_0 = 0.2$ e $r^2 = (x - x_0)^2 + (y - y_0)^2$;
- the initial datum is

$$c_0(x,y) = \begin{cases} y(0.4 - y)\frac{4}{0.4^2} & \text{if } (x,y) \in \{0\} \times [0, 0.4] \\ 1 & \text{if } (x,y) \in \partial B_r(x_0) \\ 0 & \text{otherwise.} \end{cases}$$

Numerical tests

Non-convex domain

- we used a diffusion coefficient $\nu = 10^{-3}$;
- we imposed the following Dirichlet boundary conditions :

$$b(x,y,t) = \begin{cases} y(0.4-y)\frac{4}{0.4^2} & \text{if } (x,y) \in \{0\} \times [0,0.4],\ t \in [0,T] \\ 1 & \text{if } (x,y) \in \partial B_r(x_0),\ t \in [0,T] \\ 0 & \text{on the rest of } \partial\Omega \text{ for } t \in [0,T]. \end{cases}$$

For this problem we don't have an exact solution : the simulations show a numerical solution that's coherent with our expectations, don't show any oscillation or instability near the boundary (where we used the extrapolation).

Numerical tests

Non-convex domain - mesh

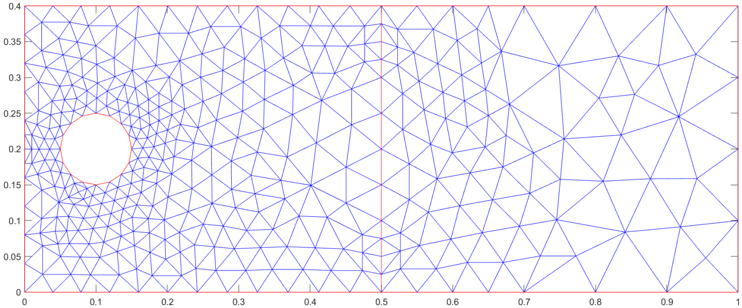


Figure – Mesh implied for the simulation

Numerical tests

Non-convex domain - velocity field

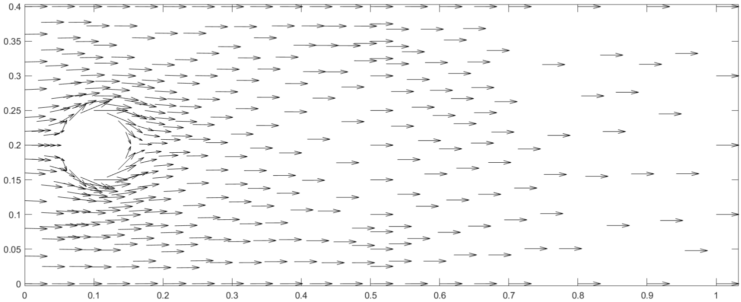
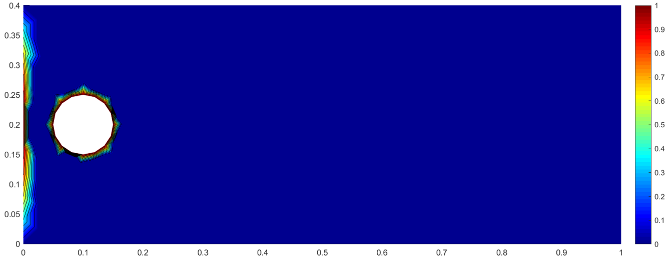


Figure – Velocity field used in the simulation

Numerical tests

Non-convex domain - video



Conclusions

- We proved that, for advection-diffusion-reaction equations, second order accuracy can be achieved using a semi-Lagrangian approach ;
- we implemented a form of boundary condition treatment that (numerically) maintains the second order ;
- everything can be generalized to systems of advection-diffusion-reaction equations ;
- in future developments, the proposed method can be extended to higher order discretizations and will be applied to the development of second order fully semi-Lagrangian methods for the Navier-Stokes equations ;
- efficiency improvement for the unstructured implementation of the scheme can be achieved [1].

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