

# B-char: an efficient (and feasible!) approach for mass-conserving characteristic schemes in 2D and 3D

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Monash Workshop on Numerical Differential Equations 2020

*Joint work with Hanz M. Cheng (formerly Monash, now Eindhoven  
University of Technology)*



**Australian Government**

**Australian Research Council**

Discrete Functional Analysis: bridging  
pure and numerical mathematics

- 1 **The problem: numerical methods with inexact calculations**
- 2 **B-char method: cheap, and perfectly mass conservative**
- 3 **Numerical tests**
  - 2D tests
  - 3D tests

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# Linear advection model

$$\begin{cases} \phi \frac{\partial c}{\partial t} + \operatorname{div}(\mathbf{u}c) = 0 & \text{on } Q_T := \Omega \times (0, T), \\ c(\cdot, 0) = c_{\text{ini}} & \text{on } \Omega. \end{cases}$$

- $\Omega$ : polygonal/polyhedral domain, with mesh  $\mathcal{M}$ .
- $\phi$ : porosity,  $0 < \phi_* \leq \phi \leq \phi^*$ , piecewise constant on mesh.
- $\mathbf{u}$ : Darcy velocity,  $\mathbf{u} \in L^\infty(0, T; L^2(\Omega))$ ,  $\operatorname{div} \mathbf{u} = 0$  and  $\mathbf{u} \cdot \mathbf{n} = 0$  on  $\partial\Omega$ .
- $c_{\text{ini}}$ : initial concentration,  $c_{\text{ini}} \in L^\infty(\Omega)$ .

# ELLAM method

**Time steps:** Time discretisation

$$0 = t^{(0)} < t^{(1)} < \dots < t^{(N)} = T, \quad \text{with } \delta t^{(n+\frac{1}{2})} = t^{(n+1)} - t^{(n)}.$$

Let  $\mathbf{u}^{(n+1)} \in L^2(\Omega)^d$  approximate  $\mathbf{u}$  on  $(t^{(n)}, t^{(n+1)})$ , with  $\operatorname{div} \mathbf{u}^{(n+1)} = 0$  and  $\mathbf{u}^{(n+1)} \cdot \mathbf{n} = 0$  on  $\partial\Omega$ .

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**Test function:**  $\psi$  satisfying

$$\phi \frac{\partial \psi}{\partial t} + \mathbf{u}^{(n+1)} \cdot \nabla \psi = 0 \quad \text{on } \Omega \times (t^{(n)}, t^{(n+1)}), \quad \psi(\cdot, t^{(n+1)}) \text{ given.}$$

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► Set  $F_t(x)$  flow of  $\mathbf{u}^{(n+1)}/\phi$ , that is

$$\frac{dF_t(x)}{dt} = \frac{\mathbf{u}^{(n+1)}(F_t(x))}{\phi(F_t(x))}, \quad F_0(x) = x.$$

Then

$$\psi(x, t^{(n)}) = \psi(F_{\delta t^{(n+\frac{1}{2})}}(x), t^{(n+1)}).$$

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**Time stepping in ELLAM** (=Eulerian Lagrangian Localised Adjoint Method):

$$\int_{\Omega} \phi(x)(c\psi)(x, t^{(n+1)}) dx = \int_{\Omega} \phi(x)(c\psi)(x, t^{(n)}) dx$$



# ELLAM method: global and local mass conservation

**Global mass conservation:** make  $\psi(x, t^{(n+1)}) \equiv 1$ :

$$\int_{\Omega} \phi(x) c(x, t^{(n+1)}) dx = \int_{\Omega} \phi(x) c(x, t^{(n)}) dx.$$

**Local mass conservation:** since  $\operatorname{div} \mathbf{u} = 0$ ,

$$\text{If } c(\cdot, t^{(n)}) = 1 \text{ then } c(\cdot, t^{(n+1)}) = 1.$$

# ELLAM for piecewise constant approximations

- ▶ At each time, we are looking for  $c_h(\cdot, t^{(n)}) = (c_M^{(n)})_{M \in \mathcal{M}}$  piecewise constant approximation of  $c$  on  $\mathcal{M}$ .
- ▶ Notation: the porous volume in a set  $A$  is

$$|A|_\phi = \int_A \phi.$$

**ELLAM formulation:** take  $\psi(\cdot, t^{(n+1)}) = \mathbf{1}_K$  for a cell  $K \in \mathcal{M}$ :

$$|K|_\phi c_K^{(n+1)} = \sum_{M \in \mathcal{M}} |M \cap F_{-\delta t^{(n+\frac{1}{2})}}(K)|_\phi c_M^{(n)}.$$

# Global and local mass conservation

$$|K|_{\phi} c_K^{(n+1)} = \sum_{M \in \mathcal{M}} |M \cap F_{-\delta t^{(n+\frac{1}{2})}}(K)|_{\phi} c_M^{(n)}.$$

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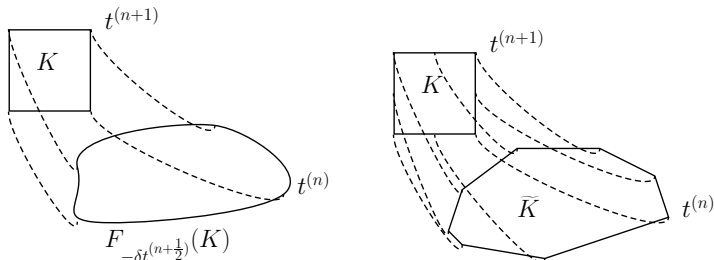
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**Local mass conservation:** OK because

$$\sum_{M \in \mathcal{M}} |M \cap F_{-\delta t^{(n+\frac{1}{2})}}(K)|_{\phi} = |F_{-\delta t^{(n+\frac{1}{2})}}(K)|_{\phi} = |K|_{\phi}.$$

# ELLAM in practice: what needs to be computed

**Transport of cells:**  $K$  polygonal/polyhedral cell, but  $F_{-\delta t^{(n+\frac{1}{2})}}(K)$  is a generic potato, that needs to be approximated...



**Figure:** Exact (left) and approximated (right) trace-back of  $K$ .

**Intersection of regions:** need to compute (porous volume of)  
 $M \cap F_{-\delta t^{(n+\frac{1}{2})}}(K).$

- ▶ Algorithms for areas of intersections of polygons (2D) are ok, but expensive.
- ▶ Algorithms for volume of intersections of polyhedras (3D) are terrible!

# ELLAM in practice: revisiting mass conservation

- ▶ Global and local mass conservation are based on

$$\sum_{K \in \mathcal{M}} |M \cap F_{-\delta t^{(n+\frac{1}{2})}}(K)|_{\phi} = |M|_{\phi} \quad (\text{global}),$$

$$\sum_{M \in \mathcal{M}} |M \cap F_{-\delta t^{(n+\frac{1}{2})}}(K)|_{\phi} = |F_{-\delta t^{(n+\frac{1}{2})}}(K)|_{\phi} = |K|_{\phi} \quad (\text{local}).$$

- ▶ Issue: we only compute  $\widehat{K}$ , and

$$|M \cap \widehat{K}|_{\phi} \approx |M \cap F_{-\delta t^{(n+\frac{1}{2})}}(K)|_{\phi}.$$

*Not a problem for global mass conservation (as  $(\widehat{K})_{K \in \mathcal{M}}$  forms a partition of the domain), but **breaks down local mass conservation...***

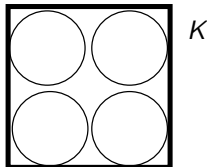


# Plan

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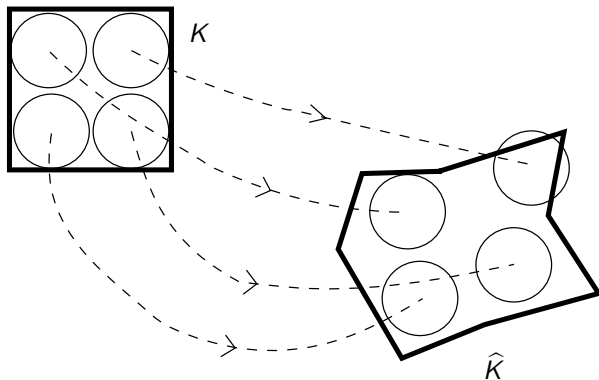
# An original idea...

Approximate polygons/polyhedras by balls,



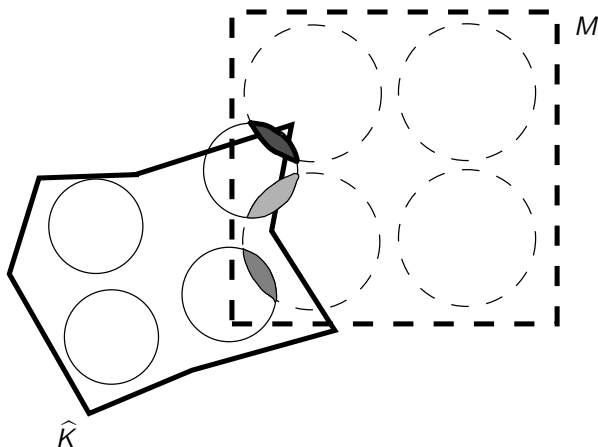
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Approximate polygons/polyhedras by balls, track balls (keeping them as balls),



# An original idea...

Approximate polygons/polyhedras by balls, track balls (keeping them as balls), intersect balls.



## ... that needs to be enhanced!

- ▶ Loss of volume in  $K$  when approximating by balls (gaps), and loss of volume when intersecting balls.
  - ▶ Very inaccurate approximation of  $\widehat{K}$  (and thus of  $F_{-\delta t^{(n+\frac{1}{2})}}(K)$ ) by tracked balls.
- ↪ bad solutions, clearly not conserving mass.

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**Distribution of porous volume:** introduce *porous density*  $\rho_K$ , constant during evolution, such that

$$\rho_K \sum_{s=1}^{n_K} |B_{K,s}|_\phi = |K|_\phi.$$

- ▶  $\rho_K |B_{K,s}|_\phi$  *equivalent* porous volume inside ball.

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**Tracking of balls:** assuming  $\phi$  constant, the volume (and radius) of  $B_{K,s}$  remains constant during tracking (*generalised Liouville theorem*).



# Initial adjustments

**Intersections of balls without loss of mass:** straight intersection of balls in  $\widehat{K}$  and  $M$  leads to

$$|\widehat{K} \cap M|_\phi \approx \sum_s \sum_m \rho_M \phi_M |\widehat{B}_{K,s} \cap B_{M,m}|.$$

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► But loss of mass through intersection of balls. So we compute the fraction of mass of  $\widehat{B}_{K,s}$  that comes from  $B_{M,m}$ :

$$f_{K,s,M,m} = \frac{\rho_M \phi_M |\widehat{B}_{K,s} \cap B_{M,m}|}{\sum_{L \in \mathcal{M}} \sum_{\ell=1}^{n_L} \rho_L \phi_L |\widehat{B}_{K,s} \cap B_{L,\ell}|}$$

and we set

$$|M \cap \widehat{K}|_\phi \approx V_{\widehat{K},M} = \sum_{s=1}^{n_K} \rho_K \widehat{\phi}_{K,s} |\widehat{B}_{K,s}| \sum_{m=1}^{n_M} f_{K,s,M,m}.$$

# Mass conservations?

**Local mass conservation:** came from

$$\sum_M |M \cap F_{-\delta t^{(n+\frac{1}{2})}}(K)|_\phi = |F_{-\delta t^{(n+\frac{1}{2})}}(K)|_\phi = |K|_\phi.$$

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We therefore need

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**OK** because  $\sum_M \sum_m f_{K,s,M,m} = 1$ .

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$$\sum_K V_{\widehat{K},M} = |M|_\phi. \quad \text{KO!}$$

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- ▶ Step 0: set  $V_{\hat{K},M}^{(0)} = V_{\hat{K},M}$ .



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For  $n = 0, \dots, N$ , iterate:

- ▶ Step 1: redistribute to get global mass conservation

$$V_{\hat{K},M}^{(n+\frac{1}{2})} = \frac{|M|_\phi}{\sum_R V_{\hat{R},M}^{(n)}} V_{\hat{K},M}^{(n)}.$$

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- ▶ Step 2: redistribute to get local mass conservation

$$V_{\hat{K},M}^{(n+1)} = \frac{|K|_\phi}{\sum_L V_{\hat{K},L}^{(n+\frac{1}{2})}} V_{\hat{K},M}^{(n+\frac{1}{2})}.$$

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**Achieving exact conservation:** after  $n \sim 10$ , stop iterations and find, in the vicinity of the current  $(V_{\hat{K},M}^{(n)})_{K,M}$ , one solution to the global and local mass conservation equations.

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**Achieving exact conservation:** after  $n \sim 10$ :

Find  $\mathbf{x} = (x_{\widehat{K},M})_{K,M}$  such that:

- $((1 + x_{\widehat{K},M})V_{\widehat{K},M}^{(n)})_{K,M}$  exactly satisfies the global and local mass balance equations,
- $0 \leq 1 + x_{\widehat{K},M} \leq 2$ ,
- $|\mathbf{x}|^2$  is minimal.

Then, use  $V_{\widehat{K},M} = (1 + x_{\widehat{K},M})V_{\widehat{K},M}^{(n)}$  as porous volumes of cell intersections.

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►  $(x_{\widehat{K},M})_{K,M}$  are  $\# \text{cells} \times \# \text{cells}$  unknowns, but the actual minimisation problem is much smaller (only a few  $V_{\widehat{K},M}^{(n)}$  are non-zero).

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## Comparison with “polygonal” ELLAM: translation

▶ “Polygonal” ELLAM: classical approach, computing  $\widehat{K}$  and intersection  $M \cap \widehat{K}$ .

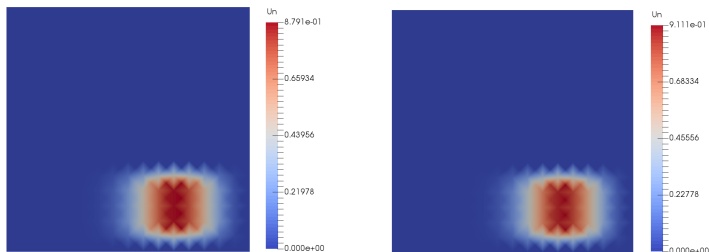
▶ B-char: 4 balls in each cell.

**Test case:**  $\Omega = (0, 1)^2$ ,  $c_{\text{ini}} = 1$  on  $(\frac{1}{16}, \frac{5}{16}) \times (\frac{1}{16}, \frac{5}{16})$ , velocity  $\mathbf{u} = (\frac{1}{16}, 0)$ , final time  $T = 8$ .

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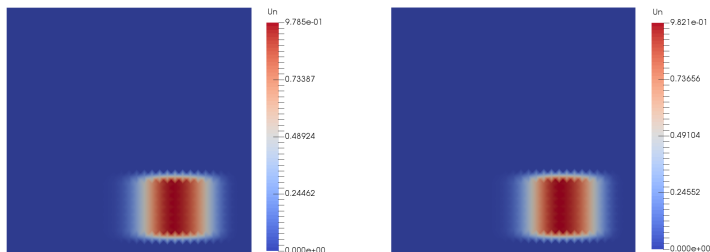


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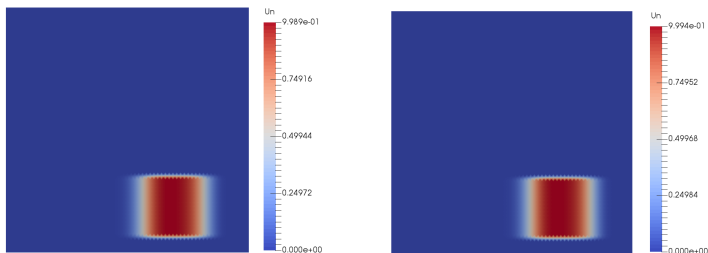


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**Figure:**  $64 \times 64$  grid,  $\delta t = 0.2$  (left: polygonal; right: B-char).

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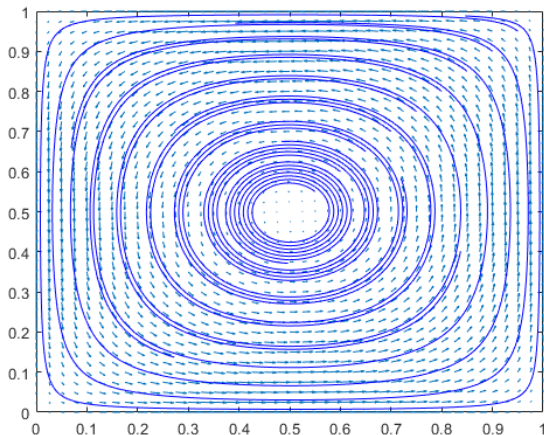
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		Polygonal		B-char	
Mesh	$\delta t$	CPU (1 step)	$L^2$ error	CPU (1 step)	$L^2$ error
$16 \times 16$	0.8	0.5s	3.7e-01	0.1s	3.8e-01
$32 \times 32$	0.4	6.5s	3.2e-01	0.4s	3.3e-01
$64 \times 64$	0.2	97.4s	2.7e-01	3.5s	2.9e-01

**Table:** CPU runtime and errors

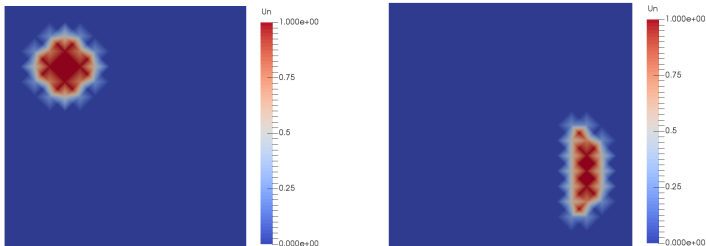
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**Test case:**  $\Omega = (0, 1)^2$ ,  $c_{\text{ini}} = 1$  on disc of center  $(\frac{1}{4}, \frac{3}{4})$  and radius  $\frac{1}{8}$ , final time  $T = 8$ . Streamlines of velocity:



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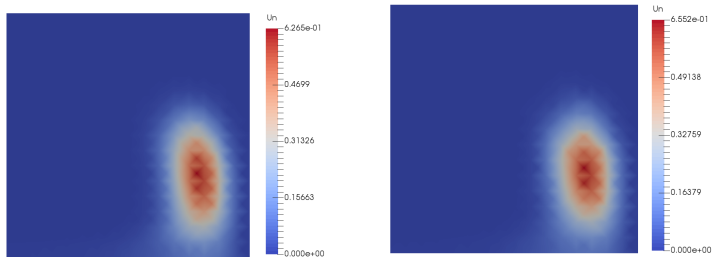
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**Figure:** Initial condition (left), final solution (right).

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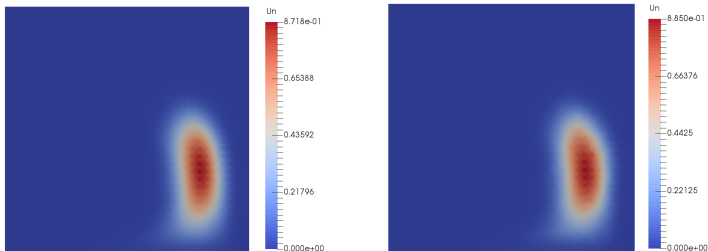


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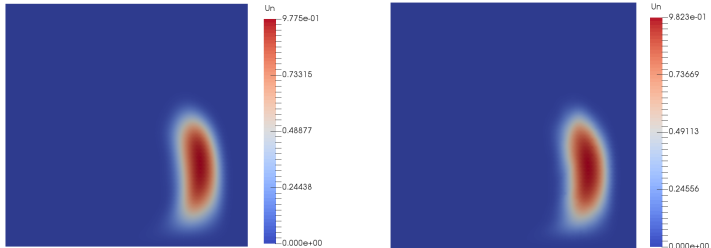
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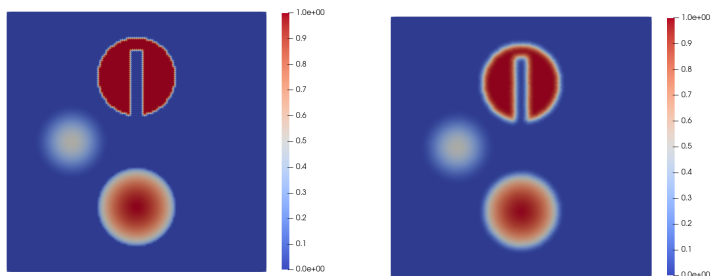
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		CPU (1 step)	$L^2$ error	CPU (1 step)	$L^2$ error
$16 \times 16$	0.8	2.7s	5.1e-01	0.2s	5.1e-01
$32 \times 32$	0.4	43s	4.2e-01	1.3s	4.1e-01
$64 \times 64$	0.2	701s	3.6e-01	14.5s	3.6e-01

**Table:** CPU runtime and errors

# Solid body rotation

**Velocity:** simple rotation around the center of  $\Omega = (0, 1)^2$ .



**Figure:** Solid body rotation on a  $128 \times 128$  mesh (left: initial condition; right: numerical solution at  $T = 2\pi$ ).

► Underlying ELLAM discretisation allows for larger time steps  $\delta t = \frac{2\pi}{10}$  (in literature, usually,  $\delta t \leq \frac{2\pi}{810}$ ).

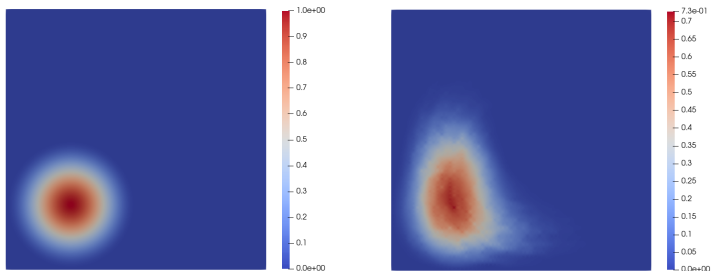
# Deformational flow

**Velocity:** velocity reverses at half-time  $T/2$ :

$$\mathbf{u} = (\sin^2(\pi x) \sin(2\pi y) \cos(\pi t/T), -\sin^2(\pi y) \sin(2\pi x) \cos(\pi t/T)).$$

# Deformational flow

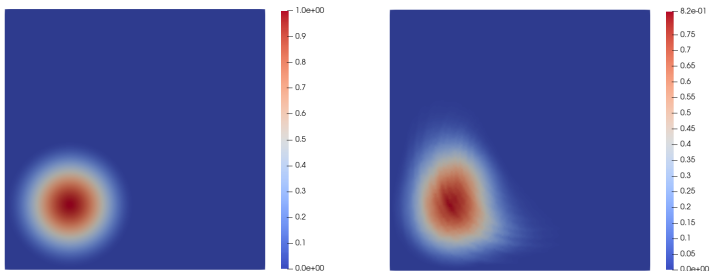
## Results:



**Figure:**  $64 \times 64$  mesh,  $\delta t = 0.5$  (left: initial condition; right: numerical solution at  $T = 5$ ).

# Deformational flow

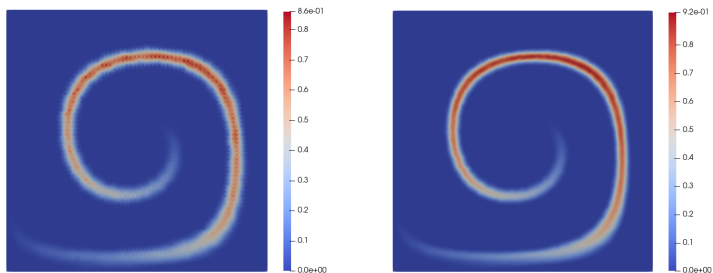
## Results:



**Figure:**  $128 \times 128$  mesh,  $\delta t = 0.25$  (left: initial condition; right: numerical solution at  $T = 5$ ).

# Deformational flow

## Results:



**Figure:** At halftime  $T = 2.5$  (left:  $64 \times 64$  cells; right:  $128 \times 128$  cells).



# Plan

- 1 The problem: numerical methods with inexact calculations
- 2 B-char method: cheap, and perfectly mass conservative
- 3 Numerical tests**
  - 2D tests
  - 3D tests

# Setting

- ▶  $\Omega = (0, 1)^3$ ,  $T = 8$ .
- ▶ B-char with 8 balls per cell,  $16^3$  mesh,  $\delta t = 0.8$ .
- ▶ 3 test cases:
  1. Piecewise constant  $c_{\text{ini}}$  in cube, velocity: translation in  $x$ .
  2. Piecewise constant  $c_{\text{ini}}$  in cylinder, velocity: rotation & stretching in  $(x, y)$ , translation in  $z$ .
  3. Continuous bump  $c_{\text{init}}$ , same velocity as in 2.

# Results

Test case	$\delta t$	CPU time (one time step)	$L^1$ error	$L^2$ error
1	0.8	37.2s	4.8e-01	4.1e-01
2	0.8	63.5s	9.6e-01	6.2e-01
3	0.8	63.2s	2.4e-01	2.4e-01

**Table:** CPU runtime and errors in 3D.

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